

SEARCH REQUEST FORM

Scientific and Technical Inf rmation Center

Requester's Full Name: PATET Art Unit: 1624 Phone No Mail Box and Bldg/Room Location:	umber 30 8 4 + 8	Examiner #: 70 Date: 4 - Serial Number: 10 0 69 Is Format Preferred (circle): PAPER DIS	29/c2 03' SK E-MAIL
If more than one search is submitted, please prioritize searches in order of need.			
Include the elected species or structures, ke	ywords, synonyms, acronyr nat may have a special mear	specifically as possible the subject matter to be ms, and registry numbers, and combine with the ning. Give examples or relevant citations, author bstract.	concept or .
Title of Invention: PHENT	L SULFA	MATE DERIVATIV	ES
Inventors (please provide full names):	1	(1 KOIZUMI et	d
Earliest Priority Eiling Date:	16/1999		
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Searcher Prep & Review Time: 40	Fulltext	Sequence Systems	
Clerical Prep Time:	Patent Family	WWW/Internet	
Online Time: 45	Othér	Other (specify)	
PTO-1590 (8-01)			

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L1 SCREEN CREATED

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Uploading C:\STNEXP4\QUERIES\10019693 (patel - amended).str

L2 STRUCTURE UPLOADED

=> que L2 NOT L1

L3 QUE L2 NOT L1

=> d 13

L3 HAS NO ANSWERS

L1 SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047 L2 STR

SQ.

Structure attributes must be viewed using STN Express query preparation. L3 $$\operatorname{QUE}$$ L2 NOT L1

=> s 13 sss sam

SAMPLE SEARCH INITIATED 17:20:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 213 TO ITERATE

100.0% PROCESSED 213 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

3385 TO 5135

PROJECTED ANSWERS: 2 TO

L4 2 SEA SSS SAM L2 NOT L1

=> s 13 sss ful

124

FULL SEARCH INITIATED 17:20:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4194 TO ITERATE

100.0% PROCESSED 4194 ITERATIONS SEARCH TIME: 00.00.01

63 ANSWERS

L5

63 SEA SSS FUL L2 NOT L1

=> s 15

L6

17 L5

=> d 16 1-17 bib, ab, hitstr

L6 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2003:312347 CAPLUS

DN 139:30177

TI Carbonic Anhydrase Inhibitors. Inhibition of Cytosolic Isozymes I and II and Transmembrane, Tumor-Associated Isozyme IX with Sulfamates Including EMATE Also Acting as Steroid Sulfatase Inhibitors

AU Winum, Jean-Yves; Vullo, Daniela; Casini, Angela; Montero, Jean-Louis; Scozzafava, Andrea; Supuran, Claudiu T.

CS Laboratoire de Chimie Biomoleculaire, UMR 5032, Ecole Nationale Superieure de Chimie de Montpellier, Université Montpellier II, Montpellier, 34296, Fr.

SO Journal of Medicinal Chemistry (2003) 46(11), 2197-2204 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

AB A series of sulfamates or bis-sulfamates incorporating aliph., arom., polycyclic (steroidal), and sugar moieties in their mols. has been synthesized and assayed as inhibitors of the zinc enzyme carbonic anhydrase (CA), and more precisely of the cytosolic isoenzymes CA I and II, and the transmembrane, tumor-assocd. isoenzymes CA IX. Some of these compds. were previously reported to act as inhibitors of steroid sulfatases, among which estrone sulfatase (ES) and dehydroepiandrosterone sulfatase (DHEAS) are the key therapeutic targets for estrogen-dependent tumors. Very potent (nanomolar) inhibitors were detected against the three investigated CA isoenzymes. Best CA I inhibitors were phenylsulfamate and some of its 4-halogeno derivs., as well as the aliph. compd. n-octyl sulfamate. Against CA II, low nanomolar inhibitors (1.1 -5 nM) were phenylsulfamate and some of its 4-halogeno/nitro derivs., n-octyl sulfamate, and estradiol 3,17.beta.-disulfamate among others. All the investigated sulfamates showed efficient CA IX inhibitory properties, with inhibition consts. in the range of 18 - 63 nM. The best CA IX inhibitor detected so far was 4-chlorophenylsulfamate. These data are crit. for the design of novel antitumor properties, mainly for hypoxic tumors that overexpress CA IX, which are nonresponsive to radiation or chemotherapy. The antitumor properties of the ES/DHEAS inhibitors in clin. trials may on the other hand also be due to their potent inhibitory properties of CA isoenzymes involved in tumorigenicity, such as CA II and CA IX.

IT 25999-01-3P, p-Biphenyl sulfamate

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(carbonic anhydrase inhibitors. inhibition of cytosolic isoenzymes I and II and transmembrane, tumor-assocd. isoenzyme IX with sulfamates including EMATE also acting as steroid sulfatase inhibitors)

RN 25999-01-3 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME) ·

L6 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2003:103675 CAPLUS

DN 139:193408

TI Design, synthesis and biochemical evaluation of AC ring mimics as novel inhibitors of the enzyme estrone sulfatase (ES)

AU Ahmed, Sabbir; James, Karen; Owen, Caroline P.

CS School of Chemical and Pharmaceutical Sciences, Kingston University, Surrey, KT1 2EE, UK

Journal of Steroid Biochemistry and Molecular Biology (2003), Volume Date 2002, 82(4-5), 425-435 CODEN: JSBBEZ; ISSN: 0960-0760

PB Elsevier Science Ltd.

DT Journal

LA English

AB We report the results of our study into a series of 4'-O-sulfamoyl-4-biphenyl based compds. as novel inhibitors of the enzyme estrone sulfatase (ES). From the results of the mol. modeling design process, it was suggested that these compds. would be able to mimic both the A and C rings of the steroid backbone, and thus possess inhibitory activity against ES. The results of the biochem. evaluation study show that these compds. are indeed good inhibitors, possessing greater inhibitory activity than COUMATE, but weaker inhibitory activity than EMATE or the tricyclic deriv. of COUMATE, namely 667-COUMATE. Furthermore, the compds. are obsd. to be irreversible inhibitors.

IT 25999-01-3P

RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and reactant; design, synthesis and biochem. evaluation of AC ring mimics as novel inhibitors of estrone sulfatase)

RN 25999-01-3 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

IT 319014-71-6P 319014-72-7P 471269-63-3P 471269-64-4P 471269-65-5P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis; design, synthesis and biochem. evaluation of AC ring mimics as novel inhibitors of estrone sulfatase)

RN 319014-71-6 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 319014-72-7 CAPLUS

CN Sulfamic acid, 4'-cyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & \\ H_2N-S-O & \\ & & \\ O & & \\ \end{array}$$

RN 471269-63-3 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 471269-64-4 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, propyl ester
(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ H_2N-S-O & & & \\ & & & \\ O & & & O \end{array}$$

RN 471269-65-5 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, butyl ester (9CI) (CA INDEX NAME)

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L6
     ANSWER 3 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN
     2003:44124 CAPLUS
AN
     138:55747
DN
     Preparation of arylsulfamates as estrone sulfatase inhibitors
TТ
IN
     Ahmed, Sabbir
PA
     BTG International Limited, UK
     Brit. UK Pat. Appl., 28 pp.
SO
     CODEN: BAXXDU
DT
     Patent
T.A
     English
FAN.CNT 1
                             DATE
     PATENT NO.
                       KIND
                                             APPLICATION NO.
                                                               DATE
                                             -----
                             20020724
ΡI
     GB 2371299
                        A1
                                             GB 2001-1220
                                                               20010117
                             20010117
PRAI GB 2001-1220
os
     MARPAT 138:55747
AB
     Title compds. [I; R1-R5 = H, Kalo, alkyl, nitro, (substituted) alkoxy,
     aryl, aryloxy, alkylamino, arylamino, COOR6, sulfamate group; .gtoreq.1 of
     R1-R5 = sulfamate group, aryl, aryloxy, or arylamino substituted with a sulfamate group; R6 = H, aryl, or alkyl], were prepd. Thus, NaH was added
     to a stirred soln. of Me 4-hydroxybenzoate (prepn. given) in DMF at
     O.degree.; after 30 min. aminosulfonyl chloride in PhMe was added and the
     reaction allowed to stir for 10 h to give 31.6% Me 4-
     [(aminosulfonyl)oxy]benzoate. The latter inhibited estrone sulfatase by
     74.7% at 50 .mu.M.
IT
     319014-71-6P, Methyl 4'-[(aminosulfonyl)oxy]-1,1'-biphenyl-4-
     carboxylate 471269-63-3P, Ethyl 4'-[(aminosulfonyl)oxy]-1,1'-
     biphenyl-4-carboxylate 471269-64-4P, Propyl 4'-
     [(aminosulfonyl)oxy]-1'-biphenyl-4-carboxylate 471269-65-5P,
     Butyl 4'-[(aminosulfonyl)oxy]-1'-biphenyl-4-carboxylate
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (prepn. of arylsulfamates as estrone sulfatase inhibitors)
RN
     319014-71-6 CAPLUS
     [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, methyl ester
CN
     (9CI) (CA INDEX NAME)
```

RN 471269-64-4 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, propyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ H_2N-S-O & & & \\ & & & \\ O & & & \\ \end{array}$$

RN 471269-65-5 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, butyl ester (9CI) (CA INDEX NAME)

L6 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2002:482277 CAPLUS

DN 138:66153

TI The design, synthesis, and biochemical evaluation of derivatives of biphenyl sulfamate-based compounds as novel inhibitors of estrone sulfatase

AU Ahmed, Sabbir; James, Karen; Owen, Caroline P.

CS School of Chemical and Pharmaceutical Sciences, Kingston University, Surrey, Kingston upon Thames, KT1 2EE, UK

SO Biochemical and Biophysical Research Communications (2002), 294(1), 180-183

CODEN: BBRCA9; ISSN: 0006-291X

PB Elsevier Science

DT Journal

LA English

OS CASREACT 138:66153

AB We report the initial results of our study into the use of a potential transition state (TS) of the reaction catalyzed by the enzyme estrone sulfatase (ES) in the design of a series of simple 4'-O-sulfamoyl-4-biphenyl-based compds. as novel inhibitors of ES. The results of the study show that these compds. are: potent inhibitors, possessing greater inhibitory activity than 4-methylcoumarin-7-O-sulfamate (COUMATE); weaker inhibitors than the tricyclic deriv. of COUMATE, namely 667-COUMATE and the steroidal inhibitor estrone-3-O-sulfamate (EMATE), and irreversible inhibitors of ES.

IT 25999-01-3P

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(design, synthesis, and biochem. evaluation of derivs. of biphenyl sulfamate-based compds. as novel inhibitors of estrone sulfatase)

RN 25999-01-3 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

IT 319014-71-6P 319014-72-7P 471269-63-3P 471269-64-4P 471269-65-5P

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(design, synthesis, and biochem. evaluation of derivs. of biphenyl sulfamate-based compds. as novel inhibitors of estrone sulfatase)

RN 319014-71-6 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 319014-72-7 CAPLUS

CN Sulfamic acid, 4'-cyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 471269-63-3 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 471269-64-4 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, propyl ester (9CI) (CA INDEX NAME)

RN 471269-65-5 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, butyl ester (9CI) (CA INDEX NAME)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2002:324919 CAPLUS

DN 137:310661

TI Design, synthesis and biochemical evaluation of AC ring mimics as novel inhibitors of the enzyme estrone sulfatase (ES)

AU Ahmed, Sabbir; James, Karen; Owen, Caroline P.: Patel, Chirag K.

CS School of Chemical and Pharmaceutical Sciences, Kingston University, Kingston upon Thames, Surrey, KT1 2EE, UK

SO Bioorganic & Medicinal Chemistry Letters (2002), 12(10), 1343-1346 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

AB 4-(4-RC6H4)C6H4O3SNH2 [= H, CN, CO2Me, CO2Et, CO2Pr, CO2Bu] were prepd.as novel inhibitors of the enzyme estrone sulfatase (ES). The results of the study show that these compds. are potent inhibitors, possessing greater inhibitory activity than coumate, but weaker inhibitory activity than emate or the tricyclic deriv. of coumate, namely 667-coumate. Furthermore, the compds. are obsd. to be irreversible inhibitors.

IT 25999-01-3P 319014-71-6P 319014-72-7P 471269-63-3P 471269-64-4P 471269-65-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and estrone sulfatase inhibiting activity of sulfamoyloxybiphenyls as steroid AC ring mimics)

RN 25999-01-3 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-71-6 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 319014-72-7 CAPLUS

CN Sulfamic acid, 4'-cyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} 0 & & \\ H_2N-S-O & & \\ 0 & & \\ \end{array}$$

RN 471269-63-3 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 471269-64-4 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, propyl ester
(9CI) (CA INDEX NAME)

RN 471269-65-5 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, butyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & \circ \\ & -S - NH_2 \\ & \circ & \circ \\ \end{array}$$

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 6 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN 1.6 AN 2002:63493 CAPLUS DN 136:112635 ΤI Biphenylyl sulfamates as steroid sulfatase inhibitors for estrogen-dependent diseases Jinbo, Yoshikazu; Miyasaka, Tomohiro; Inoue, Yoshimasa IN PA Japan Organo Co., Ltd., Japan SO Jpn. Kokai Tokkyo Koho, 14 pp. CODEN: JKXXAF DΤ Patent LА Japanese FAN.CNT 1 PATENT NO. KIND APPLICATION NO. DATE JP 2002020362 A2 20020123 JP 2000-245314 20000706 PRAI JP 2000-245314 **2**000706 MARPAT 136:112635 4-RC6H4C6H4OSO2NH2-4 [I; R = CO2H, CONR1R2, CONR1OCH2Ph, COR2, C(OH)R1R2; AB R1 = H, (un)substituted alkyl; 2 = (un)substituted alkyl] are prepd. I are useful for treatment of mammary cancer, endometrial cancer, endometriosis, uterine myoma, etc. I (R = COCH2C6H4CMe3-4) (prepn. given) inhibited human placenta-derived steroid sulfatase at IC50 3.6 .mu.M. ΙT 390358-08-4P 390358-09-5P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of biphenylyl sulfamates as steroid sulfatase inhibitors for treatment of estrogen-dependent diseases)

390358-08-4 CAPLUS

RN

CN

RN 390358-09-5 CAPLUS

CN Sulfamic acid, 4'-[[4-(1,1-dimethylethyl)phenyl]acetyl][1,1'-biphenyl]-4yl ester (9CI) (CA INDEX NAME)

Sulfamic acid, 4'-acetyl[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O & O \\ H_2N-S-O & O \\ O & C-CH_2 \end{array}$$

IT 390358-11-9P 390358-12-0P 390358-14-2P 390358-16-4P 390358-17-5P 390358-19-7P 390358-21-1P 390358-23-3P 390358-25-5P 390358-27-7P 390358-29-9P 390358-31-3P 390358-33-5P 390358-34-6P 390358-35-7P

390358-36-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of biphenylyl sulfamates as steroid sulfatase inhibitors for treatment of estrogen-dependent diseases)

RN 390358-11-9 CAPLUS

CN Sulfamic acid, 4'-(1-oxopentyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ H_2N-S-O & & & \\ & & & \\ O & & & \\ O & & & \\ \end{array}$$

RN 390358-12-0 CAPLUS

CN Sulfamic acid, 4'-(1-oxoheptyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 390358-14-2 CAPLUS

CN Sulfamic acid, 4'-[(ethylamino)carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 390358-16-4 CAPLUS

CN Sulfamic acid, 4'-[(octylamino)carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

Me- (CH₂)
$$_{7}$$
-NH-C
0
0
0
S-NH₂
0
0

RN 390358-17-5 CAPLUS

CN Sulfamic acid, 4'-[[(2-phenylethyl)amino]carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 390358-19-7 CAPLUS

CN Sulfamic acid, 4'-[[[[4-(1,1-dimethylethyl)phenyl]methyl]amino]carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O & O \\ H_2N-S-O & H_2N-C-NH-CH_2 \end{array}$$

RN 390358-21-1 CAPLUS

CN Sulfamic acid, 4'-[[[4-(1,1-dimethylethyl)phenyl]amino]carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O & O & Bu-t \\ H_2N-S-O & 0 & C-NH & C$$

RN 390358-23-3 CAPLUS

CN Sulfamic acid, 4'-[[(phenylmethoxy)amino]carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 390358-25-5 CAPLUS

CN Sulfamic acid, 4'-[[methyl(phenylmethyl)amino]carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 390358-27-7 CAPLUS

CN Sulfamic acid, 4'-[[[[4-(1,1-dimethylethyl)phenyl]methyl]methylamino]carbo nyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & Me \\ \parallel & \parallel \\ O & C-N-CH_2 \end{array}$$

RN 390358-29-9 CAPLUS

CN Sulfamic acid, 4'-[[butyl(phenylmethyl)amino]carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ H_2N-S-O & & & \\ C-N-Bu-n & & \\ & & & \\ O & & CH_2-Ph \end{array}$$

RN 390358-31-3 CAPLUS

CN Sulfamic acid, 4'-[[[[4-(1,1-dimethylethyl)phenyl]methyl]octylamino]carbon yl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & & & \\ H_2N-S-O & & & & \\ O & & & & \\ O & & & & \\ \end{array}$$

RN 390358-33-5 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]- (9CI) (CA INDEX NAME)

RN 390358-34-6 CAPLUS

CN Sulfamic acid, 4'-(1-hydroxyethyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & \circ \\ \text{Me-CH} & \circ - \text{S-NH}_2 \\ & \circ & \circ \\ \text{OH} & \circ & \circ \end{array}$$

RN 390358-35-7 CAPLUS

CN Sulfamic acid, 4'-[2-[4-(1,1-dimethylethyl)phenyl]-1-hydroxyethyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & OH & OH \\ H_2N-S-O & CH-CH_2 & CH-CH_2 \end{array}$$

RN 390358-36-8 CAPLUS

CN Sulfamic acid, 4'-[2-[4-(1,1-dimethylethyl)phenyl]-1-hydroxy-1-methylethyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & Me \\ H_2N-S-O & C-CH_2 \\ \hline O & OH \\ \end{array}$$

- L6 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN
- AN 1985:453763 CAPLUS
- DN 103:53763
- TI Biphase systems. 7. Synthesis of simple and N-substituted sulfamates under conditions of liquid-liquid phase transfer
- AU Hedayatullah, Mir; Hugueny, Jean Claude
- CS Inst. Topol. Dyn. Syst., Univ. Paris VII, Paris, 75005, Fr.
- Phosphorus and Sulfur and the Related Elements (1984), 20(3), 371-5 CODEN: PREEDF; ISSN: 0308-664X
- DT Journal
- LA French
- AB Sulfamates p-R1C6H4OSO2NR2 (R2N = H2N, piperidino, morpholino, 1-pyrrolidinyl; R1 = H, Me, C1, Ph) were prepd. by redn. of azides p-R1C6H4SO2N3 or by esterification of phenols p-R1C6H4OH with R2NSO2C1 under phase-transfer catalysis conditions.
- IT 25999-01-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
- (prepn. of)
 RN 25999-01-3 CAPLUS
- CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

L6 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1978:442661 CAPLUS

DN 89:42661

TI A convenient synthesis of aryl sulfamates

AU Hedayatullah, Mir; Guy, Alain

CS Lab. Chim. Org., Conservatoire Natl. Arts Metiers, Paris, Fr.

SO Synthesis (1978), (5), 357 CODEN: SYNTBF; ISSN: 0039-7881

DT Journal

LA English

AB RnC6H5-nO3SNH2 (Rn = H, 2-, 4-Me, 2,6-Me2, 2-, 4-Ph, 4-Cl) were prepd. in 50-75% yield by NaBH4 redn. of RnC6H5-nO3SN3.

IT 25999-01-3P 67073-77-2P

RN 25999-01-3 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 67073-77-2 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

- L6 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN
- AN 1975:547252 CAPLUS
- DN 83:147252
- TI Synthesis and reduction of aryl azidosulfates. VI
- AU Hedayatullah, Mir; Guy, Alain
- CS Lab. Chim. Org. Appl., Conservatoire Natl. Arts Metiers, Paris, Fr.
- SO Tetrahedron Letters (1975), (29), 2455-8 CODEN: TELEAY; ISSN: 0040-4039
- DT Journal
- LA French
- AB Reaction of p-RC6H4OSO2Cl (R = H, Me, Cl, Ph) with NaN3 in MeCN gave 90-8% p-RC6H4OSO2N3 (I) which in MeOH with powd. Cu gave 47-86% p-RC6H4OSO2NH2. LiAlH4 redn. of I gave the corresponding phenols by cleavage of the O-S bond.
- IT 25999-01-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

- RN 25999-01-3 CAPLUS
- CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

- L6 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN
- AN 1972:539511 CAPLUS
- DN 77:139511
- TI Preparation and reactions of aryloxysulfonyl isocyanates
- AU Lohaus, Gerhard
- CS Farbwerke Hoechst A.-G., Frankfurt/M., Fed. Rep. Ger.
- SO Chemische Berichte (1972), 105(9), 2791-9 CODEN: CHBEAM; ISSN: 0009-2940
- DT Journal
- LA German
- AB Re-action of phenols ROH (e.g. R = Ph, p-MeC6H4, m-ClC6H4, 2,4,6-Cl3C6H2, p-NCC6H4) with ClSO2NCO gave 40-79% ROSO2NCO (I). Hydrolysis of I yielded nearly quant. ROSO2NH2 (II). I are highly active compds. and the reactivity corresponded to the acidity of the starting phenols. II was useful for the transfer of SO2NH2 groups, e.g. to amines.
- IT 25999-01-3P
 - RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
- RN 25999-01-3 CAPLUS
- CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

L6 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1970:55051 CAPLUS

DN 72:55051

TI Sulfamic acid aryl esters

PA Farbwerke Hoechst A.-G

SO Fr., 3 pp.

CODEN: FRXXAK

DT Patent

LA French

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI FR 1554976 19690124 PRAI DE 19670128

AB Isocyanates Ar(OSO2NCO)n (where Ar = aryl, n = 1 or 2) (Ger. 1,230,017) react with H2O to yield aryl sulfamate N-carboxylic acids which lose CO2 spontaneously to form Ar(OSO2NH2)n (I). Thus, 15 g H2O is added dropwise to 64 g 4-NCC6H4OSO2NCO in 500 ml CCl4 to ppt. 55 g 4-NCC6H4-OSO2NH2, m. 155.degree. Other I (n = 1) prepd. are the following (Ar and m.p. given): 4-ClC6H4, 105.degree.; 3-ClC6H4, 80.degree.; Ph, 86.degree.; 4-MeC6H4, 80.degree.; 3-MeC6H4, 88.degree.; 2,6-Me2C6H3, 110.degree.; 2,3-Me2-C6H3, 78.degree.; 2,5-Me2C6H3, 104.degree.; 2,4,5-Cl3C6H2 (II), 158.degree.; 2,4,6-Cl3C6H2, 144.degree.; 2,4,6-Br3C6H2, 164.degree.; C6Cl5, 215.degree.; 4-MeO-C6H4, 165.degree.; 4-PhN2C6H4, 160.degree.; the sulfonate of 3-hydroxydibenzofuran, 156.degree.; and hydroquinone bis(sulfamate), 200.degree. The compds. are useful for transferring the sulfonamide group. Thus, by shaking 1.35 g II with 0.9 g morpholine in 5 ml CH2Cl2, the ester dissolves to yield 0.71 g morpholine-N-sulfonamide, m. 160.degree..

IT 25999-01-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 25999-01-3 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

=> d his

(FILE 'HOME' ENTERED AT 17:19:24 ON 02 OCT 2003)

FILE 'REGISTRY' ENTERED AT 17:19:37 ON 02 OCT 2003

SCREEN 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047 L1

L2 STRUCTURE UPLOADED

L3 QUE L2 NOT L1

2 S L3 SSS SAM L4

63 S L3 SSS FUL L5

FILE 'CAPLUS' ENTERED AT 17:20:32 ON 02 OCT 2003

L6 17 S L5

FILE 'CAOLD' ENTERED AT 17:21:13 ON 02 OCT 2003

=> s 15

L7 0 L5

=> log y

SINCE FILE TOTAL ENTRY SESSION 0.40 226.69 COST IN U.S. DOLLARS

FULL ESTIMATED COST

TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE

ENTRY SESSION 0.00 -11.07 CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 17:21:27 ON 02 OCT 2003

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ANSWER 7 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN
L6
     2001:31456 CAPLUS
ΑN
DN
     134:100645
ΤI
     Preparation of phenyl sulfamate derivatives as steroid sulfatase
     Koizumi, Naoyuki; Okada, Makoto; Iwashita, Shigeki; Takegawa, Shigehiro;
IN
     Nakagawa, Takayoshi; Takahashi, Hiroo; Fujii, Tomohito
     Teikoku Hormone Mfg. Co., Ltd., Japan
PA
     PCT Int. Appl., 85 pp.
SO
     CODEN: PIXXD2
DΤ
     Patent
LΑ
     Japanese
FAN.CNT 1
     PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO.
                                                            DATE
                            20010111
                                           WO 2000-JP4427
                                                            20000704
ΡI
     WO 2001002349
                      A1
         W: AU, CA, CN, JP, KR, US
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE
     JP 2002293768
                            20021009
                                           JP 1999-191632
                                                            19990706
                      A2
                            20020403
                                           EP 2000-940936
                                                            20000704
     EP 1193250
                      A1
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
PRAI JP 1999-191632
                            19990706
                       Α
    WO 2000-JP4427
                       W
                            20000704
OS
     MARPAT 134:100645
     Ph sulfamate derivs. of general formula (I) or salts thereof [wherein R1,
AB
     R2 = H, lower alkyl; R3 = H, halo, lower alkyl, OSO2NR1R2, lower
     alkanoylamino, NO2, cyano; A = (un)substituted Ph, naphthyl, pyridyl,
     2-substituted thiazol-4-yl, 3-substituted-isoxazol-5-yl,
     1-cyano-2-(optionally substituted phenyl)vinyl, 3-cyano-2-(optionally
     substituted phenyl) vinyl, X-NR4R5 (wherein X = CO, CH2; R4 = H, lower
     alkyl, optionally substituted Ph, lower alkanoyl, optionally substituted
     phenylcarbonyl, heteroarylcarbonyl, lower alkylsulfonyl, SO2NH2, etc.; R5
     = H, optionally substituted Ph or phenylcarbonyl; provisos are given); or
     R3 and A together with Ph group to which they are bonded represent
     fluoren-2-yl or 9-oxofluoren-2-yl; provided that when R3 = H, A .noteq.
     unsubstituted Ph] are prepd. These compds. exhibit an excellent steroid
     sulfatase inhibitory activity and being therefore effective in the
     prevention or treatment of diseases related to steroids including
     estrogen, e.g., mammary carcinoma, carcinoma of uterine body, endometrial
     hyperplasia, sterility, endometriosis, adenomyosis of uterus, autoimmune
     diseases, dementia, Alzheimer's disease and so on. Thus, 108 mg
     2'-biphenyl-4-ol was dissolved in DMF and stirred with under ice-cooling
     for 10 min, treated with 367 mg sulfamoyl chloride, and stirred at room
     temp. for 3 h to give 2'-nitrobiphenyl-4-yl sulfamate (II). II and
     2'-cyano-4'-nitrobiphenyl-4-yl sulfamate at 0.5 mg/kg p.o. in rats
     inhibited steroid sulfatase by 91.2 and 99.5%, resp., in liver and 94.9
     and 100%, resp., in uterus.
     319014-55-6P, 2'-Nitrobiphenyl-4-yl sulfamate 319014-56-7P
IT
     , 4'-Hydroxy-2-cyanobiphenyl-4-yl sulfamate 319014-57-8P,
     2'-Fluorobiphenyl-4-yl sulfamate 319014-59-0P,
     2'-(Trifluoromethyl)biphenyl-4-yl sulfamate 319014-60-3P,
     2'-Methylbiphenyl-4-yl sulfamate 319014-61-4P,
     Biphenyl-2,4'-diyl disulfamate 319014-62-5P,
     2'-Cyanomethylbiphenyl-4-yl sulfamate 319014-63-6P,
     3'-Fluorobiphenyl-4-yl sulfamate 319014-64-7P,
     3'-Nitrobiphenyl-4-yl sulfamate 319014-65-8P,
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3'-Cyanobiphenyl-4-yl sulfamate 319014-66-9P,
     3'-Cyanomethylbiphenyl-4-yl sulfamate 319014-67-0P,
     4'-Bromobiphenyl-4-yl sulfamate 319014-68-1P,
     4'-Chlorobiphenyl-4-yl sulfamate 319014-69-2P,
     4'-Methoxybiphenyl-4-yl sulfamate 319014-70-5P,
     4'-Nitrobiphenyl-4-yl sulfamate 319014-71-6P, Methyl
     4'-(sulfamoyloxy)-4-biphenylcarboxylate 319014-72-7P,
     4'-Cyanobiphenyl-4-yl sulfamate 319014-73-8P,
     4'-Trifluoromethylbiphenyl-4-yl sulfamate 319014-75-0P,
     4'-(Cyanomethyl)biphenyl-4-yl sulfamate 319014-76-1P,
     Biphenyl-4,4'-diyl disulfamate 319014-78-3P,
     2-Nitrobiphenyl-4,4'-diyl disulfamate 319014-79-4P,
     2',4'-Dinitrobiphenyl-4-yl sulfamate 319014-80-7P,
     2,2'-Dinitrobiphenyl-4,4'-diyl disulfamate 319014-81-8P,
     2'-Cyano-4'-nitrobiphenyl-4-yl sulfamate 319014-82-9P,
     4'-Cyano-2'-nitrobiphenyl-4-yl sulfamate 319014-83-0P,
     2',4'-Dicyanobiphenyl-4-yl sulfamate 319015-53-7P
     319015-61-7P, 3-Chlorobiphenyl-4-yl sulfamate 319015-62-8P
     , 3-Bromobiphenyl-4-yl sulfamate 319015-63-9P,
     3-Iodobiphenyl-4-yl sulfamate 319015-64-0P, 3-
     (Acetylamino)biphenyl-4-yl sulfamate 319015-66-2P,
     4'-((Methylsulfonyl)amino)biphenyl-4-yl sulfamate 319015-68-4P,
     2'-((Methylsulfonyl)amino)biphenyl-4-yl sulfamate 319015-70-8P,
     4'-(Methylsulfonyloxy)biphenyl-4-yl sulfamate 319015-80-0P,
     4'-(Sulfamoylamino)biphenyl-4-yl sulfamate 319015-81-1P,
     2'-(Sulfamoylamino)biphenyl-4-yl sulfamate 319015-86-6P,
     4'-Amino-2'-cyanobiphenyl-4-yl sulfamate 319015-87-7P,
     2'-Amino-4'-cyanobiphenyl-4-yl sulfamate
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of Ph sulfamate derivs. as steroid sulfatase inhibitors and
        drugs)
     319014-55-6 CAPLUS
RN
     Sulfamic acid, 2'-nitro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)
CN
```

RN 319014-56-7 CAPLUS
CN Sulfamic acid, 2-cyano-4'-hydroxy[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-57-8 CAPLUS

CN Sulfamic acid, 2'-fluoro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-59-0 CAPLUS

CN Sulfamic acid, 2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-60-3 CAPLUS

CN Sulfamic acid, 2'-methyl[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-61-4 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-2,4'-diyl ester (9CI) (CA INDEX NAME)

RN 319014-62-5 CAPLUS

CN Sulfamic acid, 2'-(cyanomethyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-63-6 CAPLUS

CN Sulfamic acid, 3'-fluoro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-64-7 CAPLUS

CN Sulfamic acid, 3'-nitro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-65-8 CAPLUS

CN Sulfamic acid, 3'-cyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-66-9 CAPLUS

CN Sulfamic acid, 3'-(cyanomethyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-67-0 CAPLUS

CN Sulfamic acid, 4'-bromo[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-68-1 CAPLUS

CN Sulfamic acid, 4'-chloro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-69-2 CAPLUS

CN Sulfamic acid, 4'-methoxy[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-70-5 CAPLUS

CN Sulfamic acid, 4'-nitro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-71-6 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 319014-72-7 CAPLUS

CN Sulfamic acid, 4'-cyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & \\ H_2N-S-O & & \\ & & \\ O & & \\ \end{array}$$

RN 319014-73-8 CAPLUS

CN Sulfamic acid, 4'-(trifluoromethyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$F_3C$$
 $O-S-NH_2$

RN 319014-75-0 CAPLUS

CN Sulfamic acid, 4'-(cyanomethyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-76-1 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-4,4'-diyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & O & \\ H_2N-S-O & & O-S-NH_2 \\ O & & O & O \\ \end{array}$$

RN 319014-78-3 CAPLUS

CN Sulfamic acid, 2-nitro[1,1'-biphenyl]-4,4'-diyl ester (9CI) (CA_INDEX NAME)

RN 319014-79-4 CAPLUS

CN Sulfamic acid, 2',4'-dinitro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-80-7 CAPLUS

CN Sulfamic acid, 2,2'-dinitro[1,1'-biphenyl]-4,4'-diyl ester (9CI) (CA INDEX NAME)

RN 319014-81-8 CAPLUS

CN Sulfamic acid, 2'-cyano-4'-nitro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-82-9 CAPLUS

CN Sulfamic acid, 4'-cyano-2'-nitro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-83-0 CAPLUS

CN Sulfamic acid, 2',4'-dicyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-53-7 CAPLUS

CN Sulfamic acid, 4-(1-naphthalenyl)phenyl ester (9CI) (CA INDEX NAME)

RN 319015-61-7 CAPLUS

CN Sulfamic acid, 3-chloro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-62-8 CAPLUS

CN Sulfamic acid, 3-bromo[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-63-9 CAPLUS

CN Sulfamic acid, 3-iodo[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-64-0 CAPLUS

CN Sulfamic acid, 3-(acetylamino)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-66-2 CAPLUS

CN Sulfamic acid, 4'-[(methylsulfonyl)amino][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-68-4 CAPLUS

CN Sulfamic acid, 2'-[(methylsulfonyl)amino][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-70-8 CAPLUS

CN Sulfamic acid, 4'-[(methylsulfonyl)oxy][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-80-0 CAPLUS

CN Sulfamic acid, 4'-[(aminosulfonyl)amino][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-81-1 CAPLUS

CN Sulfamic acid, 2'-[(aminosulfonyl)amino][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-86-6 CAPLUS

CN Sulfamic acid, 4'-amino-2'-cyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$H_2N$$
 O
 O
 S
 NH_2
 O

RN 319015-87-7 CAPLUS

CN Sulfamic acid, 2'-amino-4'-cyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN
- AN 1996:169243 CAPLUS
- DN 124:316749
- N-acyl sulfamic acid esters (or thioesters), N-acyl sulfonamides, and ΤI N-sulfonyl carbamic acid esters (or thioesters) as hypercholesterolemic
- Lee, Helen T.; Picard, Joseph A.; Sliskovic, Drago R.; Wierenga, Wendell IN
- PΑ Warner-Lambert Company, USA
- SO U.S., 17 pp. Cont.-in-part of U.S. Ser. No. 62,515, abandoned. CODEN: USXXAM
- DTPatent
- LΑ English
- FAN.CNT 2

	PA:	TENT NO.		KIND	DATE		APPLICATION NO.	DATE			
PI	ΙL	109431		A1	20010111		US 1994-223932 IL 1994-109431 CA 1994-2158268	19940426			
		9426702		A 1	19941124		WO 1994-US5233 NO, NZ, RU, SK				
		9468311		A1	19941212	-	GB, GR, IE, IT, LU, AU 1994-68311			SE	
	ΕP			A1	19960228		EP 1994-916734	19940511			
			BE,	CH, DE	, DK, ES,	FR,	GB, GR, IE, IT, LI,		NL,	PT,	SE
	JP	08510256		T2	19961029		HU 1995-2811 JP 1994-525674 AT 1994-916734	19940511			
	ES			Т3	19990901		ES 1994-916734				
	SK	282790		В6	20021203		SK 1995-1396 ZA 1994-3313	19940511			
	US	5633287		Α	19970527		US 1995-546967 FI 1995-5438	19951023			
PRAI	US	9504564 1993-6251	5	B2	19930514		NO 1995-4564	19951113			
		1994-2239 1994-US52									

MARPAT 124:316749 AB

os

The present invention is directed to title ACAT-inhibiting compds. R1XSO2NRCOYR2 useful for the regulation of cholesterol, methods for using them and pharmaceutical compns. thereof, wherein: X and Y are oxygen, sulfur, or (CR'R'')n wherein n is 1 to 4 and R' and R'' are each independently, e.g., H, alkyl, alkoxy or R' and R'' together form a spirocycloalkyl or a carbonyl; R is hydrogen, alkyl, or benzyl; R1 and R2 are Ph, substituted Ph, naphthyl, substituted naphthyl, an aralkyl group, an alkyl chain, adamantyl, or a cycloalkyl group. Thus, e.g., hydroxyethylation of 2,6-diisopropylbromobenzene with Li/ethylene oxide afforded 2-(2,6-diisopropylphenyl)ethanol; Jones oxidn. of the latter afforded the (2,6-diisopropylphenyl)acetic acid; conversion to the acid chloride followed by amidation with 2,6-diisopropylphenyl sulfamate afforded ArCH2CONHSO2OAr (Ar = 2,6-diisopropylphenyl) which exhibited IC50 = 9.7 .mu.M for inhibition of ACAT in vitro and -63% change in mean cholesterol levels in vivo.

ΙT 166519-18-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

10/019,693 (Patel - amended)

(N-acyl sulfamic acid esters, N-acyl sulfonamides, and N-sulfonyl carbamic acid esters as hypercholesterolemic agents)

RN 166519-18-2 CAPLUS

CN Sulfamic acid, [1,1':3',1''-terphenyl]-2'-yl ester (9CI) (CA INDEX NAME)

```
L6
    ANSWER 9 OF 17 CAPLUS COPYRIGHT 2003 ACS on STN
     1995:742595 CAPLUS
AN
DN
     123:143436
TΤ
     N-acyl sulfamic acid esters (or thioesters), n-acyl sulfonamides, and
     N-sulfonyl carbamic acid esters (or thioesters) as hypercholesterolemic
     Lee, Helen Tsenwhei; Picard, Joseph Armand; Sliskovic, Drago Robert;
TN
    Wierenga, Wendell
PA
    Warner-Lambert Co., USA
     PCT Int. Appl., 59 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
    English
FAN.CNT 2
    PATENT NO.
                     KIND DATE
                                        APPLICATION NO.
                                                          DATE
PI
    WO 9426702
                     A1 19941124
                                         WO 1994-US5233
                                                          19940511
        W: AU, CA, CZ, FI, HU, JP, KR, NO, NZ, RU, SK
        RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
                    A 19960213
                                                          19940413
    US 5491172
                                        US 1994-223932
                                                          19940511
    AU 9468311
                      A1
                           19941212
                                         AU 1994-68311
    AU 681152
                      B2
                           19970821
                                         EP 1994-916734
    EP 698010
                      A1
                           19960228
                                                          19940511
    EP 698010
                      В1
                         19990414
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
                      T2 19961029
     JP 08510256
                                         JP 1994-525674
                                                          19940511
    RU 2137756
                      C1
                         19990920
                                         RU 1995-122768
                                                          19940511
    SK 282790
                     B6 20021203
                                        SK 1995-1396
                                                          19940511
    FI 9505438
                     A 19951110
                                        FI 1995-5438
                                                          19951110
    NO 9504564
                                         NO 1995-4564
                     A 19960111
                                                          19951113
PRAI US 1993-62515
                     A
                         19930514
    US 1994-223932
                     Α
                          19940413
    WO 1994-US5233 W
                           19940511
OS
    MARPAT 123:143436
AΒ
    Compds. of formula R1XS(O2)NRCOYR2 (R = H, C1-8 alkyl, benzyl; R1, R2 =
    Ph, phenoxy, naphthyl, arylalkyl, C1-20 alkyl, etc.; X, Y = O, S, alkyl),
    or their salts, are useful for the regulation of plasma cholesterol.
    Compds. may be used for treatment of hypercholesterolemia and
    atherosclerosis. Prepn. of 48 compds. is presented.
ΤТ
     166519-18-2P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of acyl sulfamic acid esters (or thioesters), acyl
       sulfonamides, and sulfonyl carbamic acid esters (or thioesters) as
       antihypercholesterolemic agents)
RN
     166519-18-2 CAPLUS
     Sulfamic acid, [1,1':3',1''-terphenyl]-2'-yl ester (9CI) (CA INDEX NAME)
CN
```

L12 ANSWER 40 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 1963:421587 CAPLUS

DN 59:21587

OREF 59:3853b,3854a

TI Aromatic carboxylic acids

IN Juettner, Bernhard; Bennin, Anton

PA Bergwerksverband G.m.b.H.

SO 4 pp.

DT Patent

LA Unavailable

PATENT NO. KIND DATE APPLICATION NO. DATE

DE 1136687 19610420 PΙ 19620920 DE Aromatic alkyl compds. were oxidized in aq. lye with Cl in the presence of at least 50 wt.-% (calcd. on the aromatic alkyl compd.) of a Mn salt or MnO2 to give white, Cl-free aromatic carboxylic acids; the MnO2 can be re-used. Thus, Cl 55 passed within 2 hrs. into a boiling mixt. of H2O 700, NaOH 80, MnSO4 7 and p-MeC5H4CO2H 13.6, after 2 hrs. the whole cooled, the MnO2 (hydrate) filtered off, and the colorless filtrate carefully acidified (H2SO4) gave Cl-free p-C6H4(CO2H)2 (I) 14.8; using MnO2 2 wt. parts gave an oxidn. product contg. 2.1% Cl. A mixt. 12.2 of 60% p- and 40% o-MeC6H4CH2OH oxidized similarly gave I 8.5 and (by extn. of the filtrate) o-C6H4(CO2H)2 (II) 5.8 wt. parts; a mixt. of the same cmnpds. (obtained by boiling 1 hr. a mixt. of 57% p- and 43% o-CICH2C6H4Me 14 with NaOH 40 in H2O 1000) gave I 8 and II 4 wt. parts. Also prepd. were I, pyromellitic acid, and light-yellow a-naphthoic acid (crystd. several times from 30% MeOH) from p-xylene, durene, and a-methylnaphthalene, resp.

RN 101547-37-9 CAPLUS

CN Sulfamic acid, dipropyl-, 4,4'-biphenylylene ester (7CI) (CA INDEX NAME)

10/019,693 (patel)

VOJ (A)

L12	ANSWER	41	OF	42	CAPLUS	COPYRIGHT	2003	ACS
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AN 1963:421586 CAPLUS

DN 59:21586

OREF 59:3852g-h,3853a-b

TI Aryl dialkylsulfamates

IN Dunbar, Joseph E.

PA to Dow Chemical Co.

SO 4 pp.

DT Patent

LA Unavailable

PATENT NO. KIND DATE APPLICATION NO. DATE

PI US 3082238 19630319 US 19600328

The title compds. (I) have the formula Ar(OSO2NR2)n. I are useful as aquatic and terrestrial herbicides in the control of Anacharns, Lysimiachia nummularia, Salvinia rotundifolia and beratophyllum and as foliage fungicides in the control of late blight, wheat leaf rust and, cucumber powdery mildew. I are prepd. by the reaction of a phenol, Ar(OH)n with a dialkylsulfamoyl chloride R2NSO2Cl in a basic reaction medium. In an example, 15.1 g. dimethylsulfamoyl chloride was added to a stirred soln. of 20.8 g. 2,4,5-trichlorophenol in 50 ml. NEt3 at 62.degree.. The mixt. was stirred 4 hrs. while cooling to room temp., then poured into a mixt. of ice and concd. HCl to yield an oil which crystd. on standing. The sepd. solid was washed with H2O, 10% NaOH soln., and H2O to yield 2,4,5-trichlorophenyl dimethylsulfamate (II), m. 66-7.degree. (aq. EtOH). II was also prepd. using NaOH in place of NEt3. Also prepd. were: pentachlorophenyl dimethylsulfamate, m. 150-1.degree. (EtOH); 4-tert-butyl-2-chlorophenyl dimethylsulfamate, m. 36-7.degree. (EtOH); 4-nitrephenyl dimethylsulfamate, m. 123.5-4.5.degree. (EtOH); 3,5-dimethyl-4-dimethylaminophenyl dimethylsulfamate, m. 28- 9.degree. (aq. EtOH); 1-naphthyl dimethylsulfamate, m. 76-7.degree. (aq. MeOH); 2-naphthyl dimethylsulfamate, m. 72-3.degree. (EtOH); 4,4'-biphenylyl bis(dimethylsulfaniate), m. 191-2.degree. (HOAc); 2-methyl-4isopropylphenyl diethylsulfamate; 2-nitro-4-tert-butylphenyl diethylsulfamate; 4-diethylaminophenyl dibutylsulfamate, and 4,4'-biphenylyl bis(dipropylsulfamate).

IT 98176-69-3, Sulfamic acid, dimethyl-, 4,4'-biphenylylene ester (prepn. of)

RN 98176-69-3 CAPLUS

CN Sulfamic acid, dimethyl-, 4,4'-biphenylylene ester (7CI) (CA INDEX NAME)

- L12 ANSWER 30 OF 42 CAPLUS COPYRIGHT 2003 ACS
- 1981:586905 CAPLUS AN
- DN 95:186905
- Herbicidal benzamides ΤI
- PA Hodogaya Chemical Co., Ltd., Japan
- Jpn. Kokai Tokkyo Koho, 4 pp. CODEN: JKXXAF
- \mathbf{DT} Patent
- LA Japanese

FAN.	CNT I				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 56083467	A2	19810708	JP 1979-159270	19791210
	JP 62023748	B4	19870525		

- PRAI JP 1979-159270 19791210 Herbicidal benzamides I (R = halo- or alkyl-substituted alkylsulfonyloxy, alkylsulfamoyloxy) were prepd. Thus, stirring the K salt of I (R = OH) with MeSO2Cl in acetone 6 h gave 86.3% I (R = MeSO3).
- IT 79603-69-3P RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and herbicidal activity of)
- 79603-69-3 CAPLUS RN
- Sulfamic acid, dimethyl-, 4-[[(2,3-dichlorophenyl)amino]carbonyl]phenyl CN ester (9CI) (CA INDEX NAME)

10/019,693 (patel)

L12 ANSWER 40 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 1963:421587 CAPLUS

DN 59:21587

OREF 59:3853b,3854a

TI Aromatic carboxylic acids

IN Juettner, Bernhard; Bennin, Anton

PA Bergwerksverband G.m.b.H.

so 4 pp.

DT Patent

LA Unavailable

PATENT NO. KIND DATE APPLICATION NO. DATE

PI DE 1136687 19620920 DE 19610420

AB Aromatic alkyl compds. were oxidized in aq. lye with Cl in the presence of at least 50 wt.-% (calcd. on the aromatic alkyl compd.) of a Mn salt or MnO2 to give white, Cl-free aromatic carboxylic acids; the MnO2 can be re-used. Thus, Cl 55 passed within 2 hrs. into a boiling mixt. of H2O 700, NaOH 80, MnSO4 7 and p-MeC5H4CO2H 13.6, after 2 hrs. the whole cooled, the MnO2 (hydrate) filtered off, and the colorless filtrate carefully acidified (H2SO4) gave Cl-free p-C6H4(CO2H)2 (I) 14.8; using MnO2 2 wt. parts gave an oxidn. product contg. 2.1% Cl. A mixt. 12.2 of 60% p- and 40% o-MeC6H4CH2OH oxidized similarly gave I 8.5 and (by extn. of the filtrate) o-C6H4(CO2H)2 (II) 5.8 wt. parts; a mixt. of the same cmnpds. (obtained by boiling 1 hr. a mixt. of 57% p- and 43% o-CICH2C6H4Me 14 with NaOH 40 in H2O 1000) gave I 8 and II 4 wt. parts. Also prepd. were I, pyromellitic acid, and light-yellow a-naphthoic acid (crystd. several times from 30% MeOH) from p-xylene, durene, and a-methylnaphthalene, resp.

IT 101547-37-9, Sulfamic acid, dipropyl-, 4,4'-biphenylylene ester (prepn. of)

RN 101547-37-9 CAPLUS

CN Sulfamic acid, dipropyl-, 4,4'-biphenylylene ester (7CI) (CA INDEX NAME)

- L12 ANSWER 41 OF 42 CAPLUS COPYRIGHT 2003 ACS
- AN 1963:421586 CAPLUS
- DN 59:21586
- OREF 59:3852g-h,3853a-b
- Aryl dialkylsulfamates
- IN Dunbar, Joseph E.
- PA to Dow Chemical Co.
- so 4 pp.
- DTPatent
- LΑ Unavailable

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PΙ US 3082238 19630319 US 19600328

AB The title compds. (I) have the formula Ar(OSO2NR2)n. I are useful as aquatic and terrestrial herbicides in the control of Anacharns, Lysimiachia nummularia, Salvinia rotundifolia and beratophyllum and as foliage fungicides in the control of late blight, wheat leaf rust and, cucumber powdery mildew. I are prepd. by the reaction of a phenol, Ar(OH)n with a dialkylsulfamoyl chloride R2NSO2Cl in a basic reaction medium. In an example, 15.1 q. dimethylsulfamoyl chloride was added to a stirred soln. of 20.8 g. 2,4,5-trichlorophenol in 50 ml. NEt3 at 62.degree.. The mixt. was stirred 4 hrs. while cooling to room temp., then poured into a mixt. of ice and concd. HCl to yield an oil which crystd. on standing. The sepd. solid was washed with H2O, 10% NaOH soln., and H2O to yield 2,4,5-trichlorophenyl dimethylsulfamate (II), m. 66-7.degree. (aq. EtOH). II was also prepd. using NaOH in place of NEt3. Also prepd. were: pentachlorophenyl dimethylsulfamate, m. 150-1.degree. (EtOH); 4-tert-butyl-2-chlorophenyl dimethylsulfamate, m. 36-7.degree. (EtOH); 4-nitrephenyl dimethylsulfamate, m. 123.5-4.5.degree. (EtOH); 3,5-dimethyl-4-dimethylaminophenyl dimethylsulfamate, m. 28- 9.degree. (aq. EtOH); 1-naphthyl dimethylsulfamate, m. 76-7.degree. (aq. MeOH); 2-naphthyl dimethylsulfamate, m. 72-3.degree. (EtOH); 4,4'-biphenylyl bis(dimethylsulfaniate), m. 191-2.degree. (HOAc); 2-methyl-4isopropylphenyl diethylsulfamate; 2-nitro-4-tert-butylphenyl diethylsulfamate; 4-diethylaminophenyl dibutylsulfamate, and 4,4'-biphenylyl bis(dipropylsulfamate).

98176-69-3, Sulfamic acid, dimethyl-, 4,4'-biphenylylene ester IT (prepn. of)

98176-69-3 CAPLUS RN

Sulfamic acid, dimethyl-, 4,4'-biphenylylene ester (7CI) (CA INDEX NAME) CN

$$\begin{array}{c|c} O & O & O \\ \parallel & O & \parallel \\ 0 & O & S - NMe_2 \\ \parallel & O & O \end{array}$$

L12 ANSWER 30 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 1981:586905 CAPLUS

DN 95:186905

TI Herbicidal benzamides

PA Hodogaya Chemical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN. CNT 1

PAN.CNI I									
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE					
	- -								
PI JP 56083467	A2	19810708	JP 1979-159270	19791210					
JP 62023748	B4	19870525							
PRAI JP 1979-159270		19791210							

AB Herbicidal benzamides I (R = halo- or alkyl-substituted alkylsulfonyloxy, alkylsulfamoyloxy) were prepd. Thus, stirring the K salt of I (R = OH) with MeSO2Cl in acetone 6 h gave 86.3% I (R = MeSO3).

IT 79603-69-3P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and herbicidal activity of)

RN 79603-69-3 CAPLUS

CN Sulfamic acid, dimethyl-, 4-[[(2,3-dichlorophenyl)amino]carbonyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ \parallel \\ O \\ O \\ \end{array}$$

```
L12 ANSWER 24 OF 42 CAPLUS COPYRIGHT 2003 ACS
     1993:101936 CAPLUS
AN
     118:101936
DΝ
     Preparation of 2-phenyloxazoline compounds as herbicides
ΤI
     Sato, Kazuo; Kudo, Noriaki; Honma, Toyokuni; Endo, Takeshi; Shindo, 🖯
IN
     Masahiro
PA
     Sankyo Co., Ltd., Japan
     PCT Int. Appl., 143 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     Japanese
LΑ
FAN.CNT 1
     PATENT NO.
                     KIND DATE
                                          APPLICATION NO.
                                                            DATE
     _____
PΙ
     WO 9212139
                     A1
                            19920723
                                          WO 1991-JP1767
                                                            19911226
        W: AU, CA, HU, KR, PL, RO, RU, US
         RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE
     JP 05170750
                      A2
                            19930709
                                          JP 1991-340761
                                                            19911224
     JP 3294627
                      B2
                            20020624
                                          AU 1991-91075
                                                            19911226
     AU 9191075
                      A1
                            19920817
PRAI JP 1990-407871
                     Α
                            19901227
     JP 1991-279671
                     Α
                            19911025
                    Α
     WO 1991-JP1767
                            19911226
     MARPAT 118:101936
OS
     The title compds. [I; R1 = lower alkyl; R2 = lower (halo)alkyl; R3 = H,
AB
     lower alkyl, QR4 where Q = O or S; R4 = H, lower alkyl, cycloalkyl, lower
     alkenyl, lower alkynyl, acyl, lower alkoxycarbonyl, aryloxycarbonyl,
    -CONH2, SONH2, lower alkylsulfonyl, arylsulfonyl, di(lower
     alkoxy) (thio) phosphoryl, tri(lower alkyl) silyl, 5- or 6-membered satd.
     heterocyclyl contg. 1-3 same or different heteroatoms selected form O, S,
     and N; wherein R4 may be substituted; W = O, S; X = H, halo, lower alkyl,
     lower alkylthio; Y, Z = H, halo, lower alkyl, cyano] are prepd. Thus,
     24.6 mL of a soln. of 1 M (Me3Si)2Li in THF was slowly added to a soln. of
     3.59 g Et N-[4-chloro-2-fluoro-5-(2-methoxyethoxymethoxy)phenyl]carbamate
     and 2.60 g 1-bromo-3,3-dimethyl-2-butane in DMF at room temp. and the
     mixt. was stirred for 30 min, poured into H2O, and extd. with EtOAc to
     give, after silica gel chromatog., 48.4% I (R1 = R2 = Me, R3 =
     OCH2CH2CH2OMe, X = H, Y = F, Z = Cl, W = O). This at 5 g/are controlled
     91-100% Echinochloa crus-galli and Monochoria vaginalis without inflicting
     injury to rice seedlings. A total of 253 I were prepd.
IT
     145859-49-0P
     RL: AGR (Agricultural use); BAC (Biological activity or effector, except
     adverse); BSU (Biological study, unclassified); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of, as herbicide)
RN
     145859-49-0 CAPLUS
     Sulfamic acid, dimethyl-, 2-chloro-5-[4-chloro-5-(1,1-dimethylethyl)-2-oxo-
CN
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3(2H)-oxazolyl]-4-fluorophenyl ester (9CI) (CA INDEX NAME)

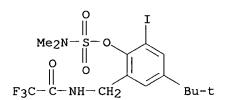
10/019,693 (patel)

L12 ANSWER 32 OF 42 CAPLUS COPYRIGHT 2003 ACS 1979:54664 CAPLUS AN 90:54664 DN Substituted 2-aminomethylphenyl sulfamates ΤI Smith, Robert L.; Stokker, Gerald E.; Cragoe, Edward J., Jr. IN PA Merck and Co., Inc., USA U.S., 6 pp. SO CODEN: USXXAM DT Patent English LА FAN.CNT 1 KIND DATE APPLICATION NO. DATE PATENT NO. ____ PΙ US 4113877 Α 19780912 US 1977-833930 19770916 DK 7804086 Α 19790317 DK 1978-4086 19780915 EP 1978-100901 19780915 EP 1266 A1 19790404 EP 1266 B119810401 R: BE, CH, DE, FR, GB, LU, NL, SE 19790424 JP 1978-114022 19780916 JP 54052056 A2 PRAI US 1977-833930 19770916 Title esters I (R = the same or different alkyl, alkoxy, aralkyl, Ph or AB halo; R1, R2 = H, C1-5 alkyl, Ph or aralkyl; n = 0-4), useful as diuretics or saluretics (no data), were prepd. by treating N-blocked 2-(aminomethyl)phenols with sulfamoyl chlorides followed by deblocking the products. Thus, 2-(aminomethyl)-4-tert-butyl-6-iodophenol was blocked by treatment with (CF3CO)20, esterified with Me2NSO2Cl, and deblocked to give I (Rn = 4-tert-Bu, 6-iodo, R1 = R2 = Me) as the hydrochloride. IT68967-69-1P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and deblocking of)

RN 68967-69-1 CAPLUS

Sulfamic acid, dimethyl-, 4-(1,1-dimethylethyl)-2-iodo-6-CN [[(trifluoroacetyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)



IT 68967-66-8P 68967-71-5P 68967-73-7P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and decarboxylation of)

RN68967-66-8 CAPLUS

Carbamic acid, [[2-[[(dimethylamino)sulfonyl]oxy]-5-(1,1-dimethylethyl)-3-CN iodophenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O \\ \parallel & \parallel \\ Me_2N-S-O \\ \parallel & O \\ I & Bu-t \end{array}$$

RN 68967-71-5 CAPLUS

CN Carbamic acid, [[3-chloro-2-[[(dimethylamino)sulfonyl]oxy]-5-(1,1-dimethylethyl)phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 68967-73-7 CAPLUS

CN Carbamic acid, [[5-(1,1-dimethylethyl)-2-[[(ethylamino)sulfonyl]oxy]-3-iodophenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 68967-67-9P 68967-72-6P 68967-74-8P

68967-76-0P 68967-77-1P 68967-78-2P

RN 68967-67-9 CAPLUS

CN Sulfamic acid, dimethyl-, 2-(aminomethyl)-4-(1,1-dimethylethyl)-6-iodophenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & I \\ \parallel & \\ Me_2N-S-O \\ \parallel & \\ O & \\ H_2N-CH_2 & Bu-t \end{array}$$

● HCl

RN 68967-72-6 CAPLUS

CN Sulfamic acid, dimethyl-, 2-(aminomethyl)-6-chloro-4-(1,1-dimethylethyl)phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & C1 \\ H_2N-CH_2 & Bu-t \end{array}$$

● HCl

RN 68967-74-8 CAPLUS

CN Sulfamic acid, ethyl-, 2-(aminomethyl)-4-(1,1-dimethylethyl)-6-iodophenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & I \\ \parallel & I \\ \hline EtNH-S-O & \\ \parallel & O \\ \hline H_2N-CH_2 & Bu-t \\ \end{array}$$

HCl

RN 68967-76-0 CAPLUS

CN Sulfamic acid, (1,1-dimethylethyl)-, 2-(aminomethyl)-4-(1,1-dimethylethyl)-6-iodophenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

10/019,693 (patel)

HCl

RN 68967-77-1 CAPLUS

CN Sulfamic acid, dimethyl-, 2-(aminomethyl)-4-(1,1-dimethylethyl)-6-iodophenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & I \\ \parallel & I \\ Me_2N-S-O & \parallel \\ O & \\ H_2N-CH_2 & Bu-t \end{array}$$

RN 68967-78-2 CAPLUS

CN Sulfamic acid, dimethyl-, 2-(aminomethyl)-4-(1,1-dimethylethyl)-6-iodophenyl ester, monohydrobromide (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O & I \\
Me_2N-S-O & I \\
O & Bu-t
\end{array}$$

● HBr

```
ANSWER 9 OF 42 CAPLUS COPYRIGHT 2003 ACS
AN
     2001:31456 CAPLUS
DN
     134:100645
     Preparation of phenyl sulfamate derivatives as steroid sulfatase
ΤI
     inhibitors
     Koizumi, Naoyuki; Okada, Makoto; Iwashita, Shigeki; Takegawa, Shigehiro;
IN
     Nakagawa, Takayoshi; Takahashi, Hiroo; Fujii, Tomohito
     Teikoku Hormone Mfg. Co., Ltd., Japan
PA
SO
     PCT Int. Appl., 85 pp.
     CODEN: PIXXD2
DΤ
     Patent
LΑ
     Japanese
FAN.CNT 1
     PATENT NO.
                      KIND
                            DATE
                                            APPLICATION NO.
                                                              DATE
PΙ
     WO 2001002349
                            20010111
                                            WO 2000-JP4427
                                                              20000704
                       A1
         W: AU, CA, CN, JP, KR, US
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE
     JP 2002293768
                       A2
                             20021009
                                            JP 1999-191632
                                                              19990706
     EP 1193250
                       A1
                            20020403
                                            EP 2000-940936
                                                              20000704
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, FI
                             19990706
PRAI JP 1999-191632
                       Α
     WO 2000-JP4427
                             20000704
                       W
     MARPAT 134:100645
os
     Ph sulfamate derivs. of general formula (I) or salts thereof [wherein R1,
AB
     R2 = H, lower alkyl; R3 = H, halo, lower alkyl, OSO2NR1R2, lower
     alkanoylamino, NO2, cyano; A = (un)substituted Ph, naphthyl, pyridyl,
     2-substituted thiazol-4-yl, 3-substituted-isoxazol-5-yl,
     1-cyano-2-(optionally substituted phenyl)vinyl, 3-cyano-2-(optionally
     substituted phenyl) vinyl, X-NR4R5 (wherein X=CO, CH2; R4=H, lower alkyl, optionally substituted Ph, lower alkanoyl, optionally substituted
     phenylcarbonyl, heteroarylcarbonyl, lower alkylsulfonyl, SO2NH2, etc.; R5
     = H, optionally substituted Ph or phenylcarbonyl; provisos are given); or
     R3 and A together with Ph group to which they are bonded represent
     fluoren-2-yl or 9-oxofluoren-2-yl; provided that when R3 = H, A .noteq.
     unsubstituted Ph] are prepd. These compds. exhibit an excellent steroid
     sulfatase inhibitory activity and being therefore effective in the
     prevention or treatment of diseases related to steroids including
     estrogen, e.g., mammary carcinoma, carcinoma of uterine body, endometrial
     hyperplasia, sterility, endometriosis, adenomyosis of uterus, autoimmune
     diseases, dementia, Alzheimer's disease and so on. Thus, 108 mg
     2'-biphenyl-4-ol was dissolved in DMF and stirred with under ice-cooling
     for 10 min, treated with 367 mg sulfamoyl chloride, and stirred at room
     temp. for 3 h to give 2'-nitrobiphenyl-4-yl sulfamate (II). II and
     2'-cyano-4'-nitrobiphenyl-4-yl sulfamate at 0.5 mg/kg p.o. in rats
     inhibited steroid sulfatase by 91.2 and 99.5%, resp., in liver and 94.9
     and 100%, resp., in uterus.
ΙT
     319014-55-6P, 2'-Nitrobiphenyl-4-yl sulfamate 319014-56-7P
      4'-Hydroxy-2-cyanobiphenyl-4-yl sulfamate 319014-57-8P,
     2'-Fluorobiphenyl-4-yl sulfamate 319014-59-0P,
     2'-(Trifluoromethyl)biphenyl-4-yl sulfamate 319014-60-3P,
     2'-Methylbiphenyl-4-yl sulfamate 319014-61-4P,
     Biphenyl-2,4'-diyl disulfamate 319014-62-5P,
     2'-Cyanomethylbiphenyl-4-yl sulfamate 319014-63-6P,
     3'-Fluorobiphenyl-4-yl sulfamate 319014-64-7P,
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3'-Nitrobiphenyl-4-yl sulfamate 319014-65-8P,

```
3'-Cyanobiphenyl-4-yl sulfamate 319014-66-9P,
3'-Cyanomethylbiphenyl-4-yl sulfamate 319014-67-0P,
4'-Bromobiphenyl-4-yl sulfamate 319014-68-1P,
4'-Chlorobiphenyl-4-yl sulfamate 319014-69-2P,
4'-Methoxybiphenyl-4-yl sulfamate 319014-70-5P,
4'-Nitrobiphenyl-4-yl sulfamate 319014-71-6P, Methyl
4'-(sulfamoyloxy)-4-biphenylcarboxylate 319014-72-7P,
4'-Cyanobiphenyl-4-yl sulfamate 319014-73-8P,
4'-Trifluoromethylbiphenyl-4-yl sulfamate 319014-75-0P,
4'-(Cyanomethyl)biphenyl-4-yl sulfamate 319014-76-1P,
Biphenyl-4,4'-diyl disulfamate 319014-78-3P,
2-Nitrobiphenyl-4,4'-diyl disulfamate 319014-79-4P,
2',4'-Dinitrobiphenyl-4-yl sulfamate 319014-80-7P,
2,2'-Dinitrobiphenyl-4,4'-diyl disulfamate 319014-81-8P,
2'-Cyano-4'-nitrobiphenyl-4-yl sulfamate 319014-82-9P,
4'-Cyano-2'-nitrobiphenyl-4-yl sulfamate 319014-83-0P,
2',4'-Dicyanobiphenyl-4-yl sulfamate 319014-84-1P,
[4-[N-Sulfamoyl-N-(4-(sulfamoyloxy)benzyl)amino]phenyl] sulfamate
319014-85-2P, [4-[N-(Methylsulfonyl)-N-(4-
(sulfamoyloxy)benzyl)amino]phenyl] sulfamate 319014-86-3P,
[4-[N-Acetyl-N-(4-(sulfamoyloxy)benzyl)amino]phenyl] sulfamate
319014-87-4P, [4-[N-Acetyl-N-(4-(sulfamoyloxy)benzyl)amino]phenyl]
acetate 319014-88-5p, [4-[N-(4-(Sulfamoyloxy)phenyl)carbamoyl]ph
enyl] sulfamate 319014-89-6P, [4-[N-Ethyl-N-(4-
(sulfamoyloxy)phenyl)carbamoyl]phenyl] sulfamate 319014-90-9P,
[4-[N-Methyl-N-(4-(sulfamoyloxy)phenyl)carbamoyl]phenyl] sulfamate
319014-91-0p, [4-[N-(3-(Sulfamoyloxy)phenyl)carbamoyl]phenyl]
sulfamate 319014-92-1P, [4-[N-Methyl-N-(3-
(sulfamoyloxy)phenyl)carbamoyl]phenyl] sulfamate 319014-93-2P
319014-95-4P 319014-97-6P 319014-99-8P,
4-(N-Phenylaminomethyl) phenyl sulfamate 319015-00-4P,
4-[N-(4-Cyanophenyl)aminomethyl]phenyl sulfamate 319015-01-5P,
4-[N-(2-Cyanophenyl)aminomethyl]phenyl sulfamate 319015-02-6P,
4-[N-(4-Hydroxyphenyl)aminomethyl]phenyl sulfamate 319015-03-7P,
4-[N-(4-Nitrophenyl)aminomethyl]phenyl sulfamate 319015-04-8P
319015-05-9P 319015-06-0P, 4-[[N,N-Bis(4-
cyanophenyl)amino]methyl]phenyl sulfamate 319015-07-1P
319015-08-2P, 4-[[N-Phenyl-N-(sulfamoyl)amino]methyl]phenyl
sulfamate 319015-09-3P, 4-[[N-(4-Cyanophenyl)-N-
(sulfamoyl)amino]methyl]phenyl sulfamate 319015-10-6P,
4-[[N-(4-Cyanophenyl)-N-nicotinoylamino]methyl]phenyl sulfamate
319015-11-7P, 4-[[N-Benzoyl-N-(4-cyanophenyl)amino]methyl]phenyl
sulfamate 319015-12-8P, 4-[[N-(4-Cyanobenzoyl)-N-(4-
cyanophenyl)amino]methyl]phenyl sulfamate 319015-13-9P,
4-(N,N-Diphenylcarbamoyl)phenyl sulfamate 319015-14-0P,
4-(N-Benzylcarbamoyl)phenyl sulfamate 319015-15-1P,
4-(N-Phenylcarbamoyl) phenyl sulfamate 319015-16-2P,
4-[[N-(4-Cyanobenzoyl)-N-methylamino]methyl]phenyl sulfamate
319015-17-3p, 4-[N-(4H-1,2,4-Triazol-4-yl)amino]methyl]phenyl
sulfamate 319015-18-4P, 4-[[N-(3-Cyanobenzoy1)-N-(4H-1,2,4-
triazol-4-yl)amino]methyl]phenyl sulfamate 319015-19-5P,
4-[[N-(4-Cyanophenyl)-N-(3-pyridyl)amino]methyl]phenyl sulfamate
319015-23-1P, 4-[[N-(4-Cyanophenyl)-N-methylamino]methyl]phenyl
sulfamate 319015-26-4P, 4-[[N-(4-Cyanophenyl)-N-
ethylamino]methyl]phenyl sulfamate 319015-30-0P,
4-[[N-(4-Cyanophenyl)-N-(2-thienylcarbonyl)amino]methyl]phenyl sulfamate
319015-34-4P, 4-[[N-(4-Cyanophenyl)-N-(3-
thienylcarbonyl)amino]methyl]phenyl sulfamate 319015-36-6P,
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4-[N-(4-Cyanophenyl)carbamoyl]phenyl sulfamate 319015-38-8P,
4-[N-(4-Cyanophenyl)-N-methylcarbamoyl]phenyl sulfamate
319015-39-9p, 4-(N',N'-Dimethylhydrazinocarbonyl)phenyl sulfamate
319015-40-2P, 2-[N-(4-(Sulfamoyloxy)phenyl)carbamoyl]phenyl
sulfamate 319015-42-4P, 3-[N-(2-(Sulfamoyloxy)phenyl)carbamoyl]p
henyl sulfamate 319015-43-5P, 3-[N-(3-
(Sulfamoyloxy)phenyl)carbamoyl}phenyl sulfamate 319015-45-7P,
3-[N-(4-(Sulfamoyloxy)phenyl)carbamoyl]phenyl sulfamate
319015-46-8P, 4-[N-(2-(Sulfamoyloxy)phenyl)carbamoyl]phenyl
sulfamate 319015-48-0P, 4-[[N-(4-Cyanophenyl)-N-(2-
pyrazinyl)amino]methyl]phenyl sulfamate 319015-50-4P
319015-52-6P 319015-53-7P 319015-54-8P,
9-Oxofluoren-2-yl sulfamate 319015-55-9p, Fluoren-2-yl sulfamate
319015-56-0P, 4-(3-Pyridyl)phenyl sulfamate 319015-57-1P
, 4-(2-Methylthiazol-4-yl)phenyl sulfamate 319015-58-2P,
4-(2-(Sulfamoyloxy)thiazol-4-yl)phenyl sulfamate 319015-60-6P,
4-[3-(N-Methylcarbamoyl)isoxazol-5-yl]phenyl sulfamate
319015-61-7P, 3-Chlorobiphenyl-4-yl sulfamate 319015-62-8P
  3-Bromobiphenyl-4-yl sulfamate 319015-63-9P,
3-Iodobiphenyl-4-yl sulfamate 319015-64-0P, 3-
(Acetylamino)biphenyl-4-yl sulfamate 319015-66-2P,
4'-((Methylsulfonyl)amino)biphenyl-4-yl sulfamate 319015-68-4P,
2'-((Methylsulfonyl)amino)biphenyl-4-yl sulfamate 319015-70-8P,
4'-(Methylsulfonyloxy)biphenyl-4-yl sulfamate 319015-72-0P
319015-74-2P 319015-76-4P 319015-78-6P,
4-[[N-(4-Cyanophenyl)-N-(2-pyrimidinyl)amino]methyl]phenyl sulfamate
319015-79-7P, 2'-Cyano-4'-nitrobiphenyl-4-yl N, N-dimethylsulfamate
319015-80-0P, 4'-(Sulfamoylamino)biphenyl-4-yl sulfamate
319015-81-1P, 2'-(Sulfamoylamino)biphenyl-4-yl sulfamate
319015-83-3P 319015-85-5P 319015-86-6P,
4'-Amino-2'-cyanobiphenyl-4-yl sulfamate 319015-87-7P,
2'-Amino-4'-cyanobiphenyl-4-yl sulfamate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
   (prepn. of Ph sulfamate derivs. as steroid sulfatase inhibitors and
   drugs)
319014-55-6 CAPLUS
Sulfamic acid, 2'-nitro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)
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RN

CN

RN 319014-57-8 CAPLUS

CN Sulfamic acid, 2'-fluoro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-59-0 CAPLUS

CN Sulfamic acid, 2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-60-3 CAPLUS

CN Sulfamic acid, 2'-methyl[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-61-4 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-2,4'-diyl ester (9CI) (CA INDEX NAME)

RN 319014-62-5 CAPLUS

CN Sulfamic acid, 2'-(cyanomethyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-63-6 CAPLUS

CN Sulfamic acid, 3'-fluoro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-64-7 CAPLUS

CN Sulfamic acid, 3'-nitro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-65-8 CAPLUS

CN Sulfamic acid, 3'-cyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-66-9 CAPLUS

CN Sulfamic acid, 3'-(cyanomethyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-67-0 CAPLUS

CN Sulfamic acid, 4'-bromo[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-68-1 CAPLUS

CN Sulfamic acid, 4'-chloro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-69-2 CAPLUS

CN Sulfamic acid, 4'-methoxy[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$H_2N-S-O$$
 OMe

RN 319014-70-5 CAPLUS

CN Sulfamic acid, 4'-nitro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{O}_2\text{N} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 319014-71-6 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 319014-72-7 CAPLUS

CN Sulfamic acid, 4'-cyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-73-8 CAPLUS

CN Sulfamic acid, 4'-(trifluoromethyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-75-0 CAPLUS

CN Sulfamic acid, 4'-(cyanomethyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$H_2N-S-O$$
 CH_2-CN

RN 319014-76-1 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-4,4'-diyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \circ & \circ & \circ \\ \parallel & \circ & \circ \\ \parallel & \circ & \circ \\ \end{array}$$

RN 319014-78-3 CAPLUS

CN Sulfamic acid, 2-nitro[1,1'-biphenyl]-4,4'-diyl ester (9CI) (CA INDEX NAME)

RN 319014-79-4 CAPLUS

CN Sulfamic acid, 2',4'-dinitro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-80-7 CAPLUS

CN Sulfamic acid, 2,2'-dinitro[1,1'-biphenyl]-4,4'-diyl ester (9CI) (CA INDEX NAME)

RN 319014-81-8 CAPLUS

CN Sulfamic acid, 2'-cyano-4'-nitro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-82-9 CAPLUS

CN Sulfamic acid, 4'-cyano-2'-nitro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-83-0 CAPLUS

CN Sulfamic acid, 2',4'-dicyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-84-1 CAPLUS

CN Sulfamic acid, 4-[[(aminosulfonyl)[4-[(aminosulfonyl)oxy]phenyl]amino]meth

yl]phenyl ester (9CI) (CA INDEX NAME)

RN 319014-85-2 CAPLUS

CN Sulfamic acid, 4-[[[4-[(aminosulfonyl)oxy]phenyl]methyl](methylsulfonyl)am ino]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O & O & O \\
H_2N - S - O & O & S - Me \\
O & N - CH_2 & O \\
\end{array}$$

RN 319014-86-3 CAPLUS

$$\begin{array}{c|c} O & O & O \\ \parallel & & \parallel & \\ H_2N-S-O & \parallel & \\ \parallel & & O & \\ \parallel & & & \\ O & & & N-CH_2 & \\ \end{array}$$

RN 319014-87-4 CAPLUS

CN Sulfamic acid, 4-[[acetyl[4-(acetyloxy)phenyl]amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

RN 319014-88-5 CAPLUS

CN Sulfamic acid, 4-[[4-[(aminosulfonyl)oxy]benzoyl]amino]phenyl ester (9CI) (CA INDEX NAME)

RN 319014-89-6 CAPLUS

CN Sulfamic acid, 4-[[4-[(aminosulfonyl)oxy]benzoyl]ethylamino]phenyl ester (9CI) (CA INDEX NAME)

RN 319014-90-9 CAPLUS

CN Sulfamic acid, 4-[[4-[(aminosulfonyl)oxy]benzoyl]methylamino]phenyl ester (9CI) (CA INDEX NAME)

RN 319014-91-0 CAPLUS

CN Sulfamic acid, 3-[[4-[(aminosulfonyl)oxy]benzoyl]amino]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & & & & & & & & & \\ & & & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & \\ & & \\ &$$

RN 319014-92-1 CAPLUS

CN Sulfamic acid, 3-[[4-[(aminosulfonyl)oxy]benzoyl]methylamino]phenyl ester (9CI) (CA INDEX NAME)

RN 319014-93-2 CAPLUS

CN Benzoic acid, 4-[(aminosulfonyl)oxy]-, 2-acetyl-1-phenylhydrazide (9CI) (CA INDEX NAME)

RN 319014-95-4 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)-4H-1,2,4-triazol-4-ylamino]methyl]phenyl ester (9CI) (CA INDEX NAME)

RN 319014-97-6 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)-4H-1,2,4-triazol-4-ylamino]carbonyl]phenyl ester (9CI) (CA INDEX NAME)

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$$\begin{array}{c|c}
N & N & CN \\
N & N & CN \\
N & C & O
\end{array}$$

$$H_2N - S - O$$

$$O$$

RN 319014-99-8 CAPLUS

CN Sulfamic acid, 4-[(phenylamino)methyl]phenyl ester (9CI) (CA INDEX NAME)

RN 319015-00-4 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ H_2N - S - O & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 319015-01-5 CAPLUS

CN Sulfamic acid, 4-[[(2-cyanophenyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

RN 319015-02-6 CAPLUS

CN Sulfamic acid, 4-[[(4-hydroxyphenyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & CH_2-NH \\ \parallel & OH \\ \parallel & O \end{array}$$

RN 319015-03-7 CAPLUS

$$\begin{array}{c|c} O & CH_2-NH \\ H_2N-S-O & NO_2 \\ 0 & \\ \end{array}$$

RN 319015-04-8 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)(4-methoxyphenyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} & & & \\ & & & \\ \text{NC} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 319015-05-9 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)phenylamino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & & & & & & \\ \text{NC} & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\$$

RN 319015-06-0 CAPLUS

CN Sulfamic acid, 4-[[bis(4-cyanophenyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

RN 319015-07-1 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)-4-pyridinylamino]methyl]phenyl ester (9CI) (CA INDEX NAME)

RN 319015-08-2 CAPLUS

CN Sulfamic acid, 4-[[(aminosulfonyl)phenylamino]methyl]phenyl ester (9CI) (CA INDEX NAME)

RN 319015-09-3 CAPLUS

CN Sulfamic acid, 4-[[(aminosulfonyl)(4-cyanophenyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$NC$$
 $O = S - NH_2$ $O - S - NH_2$ $O - S - NH_2$ $O - S - NH_2$

RN 319015-10-6 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)(3-pyridinylcarbonyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ \end{array}$$

RN 319015-11-7 CAPLUS

CN Sulfamic acid, 4-[[benzoyl(4-cyanophenyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

RN 319015-12-8 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanobenzoyl)(4-cyanophenyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & &$$

RN 319015-13-9 CAPLUS

CN Sulfamic acid, 4-[(diphenylamino)carbonyl]phenyl ester (9CI) (CA INDEX

NAME)

$$\begin{array}{c|c} C & C & C \\ H_2N - S - O & C \\ 0 & C \\ 0 & C \end{array}$$

RN 319015-14-0 CAPLUS

CN Sulfamic acid, 4-[[(phenylmethyl)amino]carbonyl]phenyl ester (9CI) (CA INDEX NAME)

RN 319015-15-1 CAPLUS

CN Sulfamic acid, 4-[(phenylamino)carbonyl]phenyl ester (9CI) (CA INDEX NAME)

RN 319015-16-2 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanobenzoyl)methylamino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{NC} & \text{O} & \text{Me} \\ \hline & \text{O} & \text{Me} \\ \hline & \text{C} - \text{N} - \text{CH}_2 \\ \end{array} \quad \begin{array}{c|c} \text{O} & \text{S} - \text{NH}_2 \\ \hline & \text{O} \\ \end{array}$$

RN 319015-17-3 CAPLUS

CN Sulfamic acid, 4-[(4H-1,2,4-triazol-4-ylamino)methyl]phenyl ester (9CI)

(CA INDEX NAME)

RN 319015-18-4 CAPLUS

CN Sulfamic acid, 4-[[(3-cyanobenzoyl)-4H-1,2,4-triazol-4-ylamino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} N \\ N \\ N \\ N \\ C \\ C \\ O \end{array}$$

$$\begin{array}{c} O \\ \parallel \\ O \\ S \\ NH_2 \\ O \\ \end{array}$$

$$\begin{array}{c} O \\ \parallel \\ O \\ \end{array}$$

RN 319015-19-5 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)-3-pyridinylamino]methyl]phenyl ester (9CI) (CA INDEX NAME)

RN 319015-23-1 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)methylamino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & \\ \text{NC} & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\$$

RN 319015-26-4 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)ethylamino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & \\ \text{NC} & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\ &$$

RN 319015-30-0 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)(2-thienylcarbonyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

RN 319015-34-4 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)(3-thienylcarbonyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
S \\
O = C \\
N \\
CH_2
\end{array}$$

$$\begin{array}{c|c}
CN \\
H_2N - S \\
O \\
O
\end{array}$$

RN 319015-36-6 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)amino]carbonyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ H_2N-S-O \\ O \\ O \\ C-NH \end{array}$$

RN 319015-38-8 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)methylamino]carbonyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ H_2N-S-O & O & Me \\ \hline \\ O & & CN \end{array}$$

RN 319015-39-9 CAPLUS

CN Benzoic acid, 4-[(aminosulfonyl)oxy]-, 2,2-dimethylhydrazide (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & &$$

RN 319015-40-2 CAPLUS

CN Sulfamic acid, 4-[[2-[(aminosulfonyl)oxy]benzoyl]amino]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
0 & NH - C \\
H_2N - S - O & H_2N - S - O \\
O & O & O & O
\end{array}$$

RN 319015-42-4 CAPLUS

CN Sulfamic acid, 2-[[3-[(aminosulfonyl)oxy]benzoyl]amino]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & O \\ H_2N-S-O & & & C \\ \hline \\ O & & & NH \\ \hline \\ O & & & \\ \\ H_2N-S-O \\ \hline \\ O & & \\ \end{array}$$

RN 319015-43-5 CAPLUS

CN Sulfamic acid, 3-[[3-[(aminosulfonyl)oxy]benzoyl]amino]phenyl ester (9CI) (CA INDEX NAME)

RN 319015-45-7 CAPLUS

CN Sulfamic acid, 4-[[3-[(aminosulfonyl)oxy]benzoyl]amino]phenyl ester (9CI)

(CA INDEX NAME)

RN 319015-46-8 CAPLUS

CN Sulfamic acid, 2-[[4-[(aminosulfonyl)oxy]benzoyl]amino]phenyl ester (9CI) (CA INDEX NAME)

RN 319015-48-0 CAPLUS

RN 319015-50-4 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)(2-thienylmethyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

RN 319015-52-6 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)(3-thienylmethyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$CH_2$$
 CH_2
 CH_2

RN 319015-53-7 CAPLUS

CN Sulfamic acid, 4-(1-naphthalenyl)phenyl ester (9CI) (CA INDEX NAME)

RN 319015-54-8 CAPLUS

CN Sulfamic acid, 9-oxo-9H-fluoren-2-yl ester (9CI) (CA INDEX NAME)

RN 319015-55-9 CAPLUS

CN Sulfamic acid, 9H-fluoren-2-yl ester (9CI) (CA INDEX NAME)

RN 319015-56-0 CAPLUS

CN Sulfamic acid, 4-(3-pyridinyl)phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ \parallel & & & \\ H_2N-S-O & & & \\ & & & \\ O & & & \\ \end{array}$$

RN 319015-57-1 CAPLUS

CN Sulfamic acid, 4-(2-methyl-4-thiazolyl)phenyl ester (9CI) (CA INDEX NAME)

RN 319015-58-2 CAPLUS

CN Sulfamic acid, 4-[4-[(aminosulfonyl)oxy]phenyl]-2-thiazolyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & \\ & & & & & \\ H_2N-S-O & & & & \\ & & & & & \\ O & & S & & & \\ \end{array}$$

RN 319015-60-6 CAPLUS

CN Sulfamic acid, 4-[3-[(methylamino)carbonyl]-5-isoxazolyl]phenyl ester (9CI) (CA INDEX NAME)

RN 319015-61-7 CAPLUS

CN Sulfamic acid, 3-chloro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-62-8 CAPLUS

CN Sulfamic acid, 3-bromo[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-63-9 CAPLUS

CN Sulfamic acid, 3-iodo[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-64-0 CAPLUS

CN Sulfamic acid, 3-(acetylamino)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-66-2 CAPLUS

CN Sulfamic acid, 4'-[(methylsulfonyl)amino][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-68-4 CAPLUS

CN Sulfamic acid, 2'-[(methylsulfonyl)amino][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-70-8 CAPLUS

CN Sulfamic acid, 4'-[(methylsulfonyl)oxy][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-72-0 CAPLUS

CN Sulfamic acid, 4-[(1Z)-2-cyano-2-phenylethenyl]phenyl ester, (.alpha.Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 319015-74-2 CAPLUS

CN Sulfamic acid, [(1Z)-1-cyano-1,2-ethenediyl]di-4,1-phenylene ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 319015-76-4 CAPLUS

CN Sulfamic acid, 4-[(1Z)-1-cyano-2-phenylethenyl]phenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 319015-78-6 CAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)-2-pyrimidinylamino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & \\ & & & & & & \\ NC & & & NM & & & \\ & & & & N-CH_2 & & & \\ & & & & & & \\ \end{array}$$

RN 319015-79-7 CAPLUS

CN Sulfamic acid, dimethyl-, 2'-cyano-4'-nitro[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-80-0 CAPLUS

CN Sulfamic acid, 4'-[(aminosulfonyl)amino][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \circ & \circ & \circ \\ \parallel & \parallel & \circ \\ \parallel & \circ & \circ \\ \downarrow & \circ & \bullet \\ \downarrow & \circ & \circ \\ \downarrow & \bullet & \circ \\ \downarrow & \circ & \circ$$

RN 319015-81-1 CAPLUS

CN Sulfamic acid, 2'-[(aminosulfonyl)amino][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319015-83-3 CAPLUS

CN Sulfamic acid, 4-[(1Z)-2-[4-[(aminosulfonyl)amino]phenyl]-2-cyanoethenyl]phenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 319015-85-5 CAPLUS

CN Benzoic acid, 4-[(1Z)-2-[4-[(aminosulfonyl)oxy]phenyl]-2-cyanoethenyl]-, methyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 319015-86-6 CAPLUS

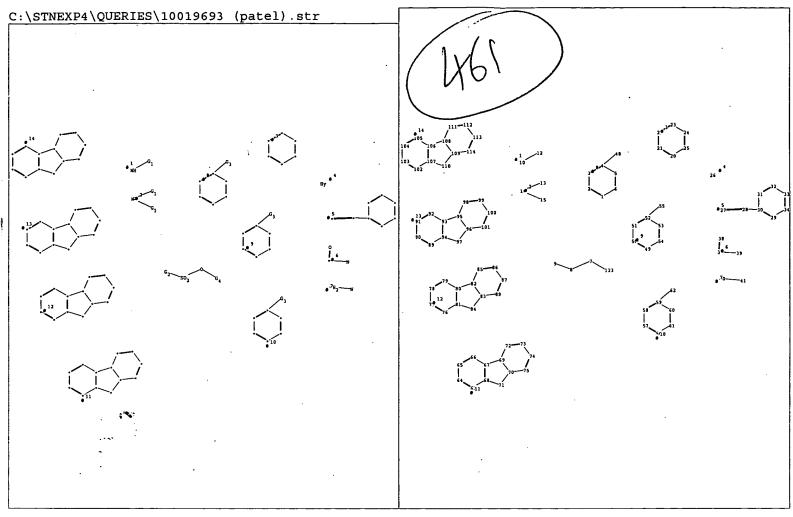
CN Sulfamic acid, 4'-amino-2'-cyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CN} & \text{O} & . \\ \text{H}_2\text{N} & \text{O} & . \\ \text{O} & \text{S} - \text{NH}_2 \\ \text{O} & \text{O} \end{array}$$

RN 319015-87-7 CAPLUS

CN Sulfamic acid, 2'-amino-4'-cyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT



```
chain nodes :
   7 8 9 10 12 13 15 16
                            26
                                27
                                   28 37 38 39 40 41 48 55 62
ring nodes :
                                24 25 29 30 31 32 33 34 49 50 51 52 53
            5 6 20
                      21 22 23
   56 57 58 59 60 61 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79
                   85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101
   80 81 82 83 84
   102 103 104 105 106 107 108 109 110 111 112 113
                                                       114
chain bonds :
   4-48 7-8 7-123 8-9 10-12 13-16 15-16 27-28 28-30 37-38 37-39 40-41 52-55
                                                                              59-62
ring bonds :
           2-3 3-4 4-5 5-6 20-21 20-25 21-22 22-23 23-24 24-25 29-30 29-34
   1-2 1-6
         32-33 33-34 49-50 49-54 50-51 51-52 52-53 53-54 56-57 56-61 57-58 58-59
         60-61 63-64
   59-60
                     63-68
                           64-65
                                 65-66 66-67
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                                                    67-69
                                                          68-71 69-70
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   104-105 105-106 106-107 106-108 107-110 108-109 108-111 109-110 109-114 111-112
   112-113 113-114
exact/norm bonds :
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   69-72 70-71 70-75 72-73 73-74 74-75 80-82 81-84 82-83 82-85 83-84 83-88 85-86
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   107-110 108-109 108-111 109-110 109-114 111-112 112-113 113-114
exact bonds :
   27-28 28-30
              40-41
normalized bonds :
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                3-4 4-5 5-6 20-21 20-25 21-22 22-23 23-24 24-25 29-30 29-34 30-31
   31-32 32-33 33-34 49-50 49-54 50-51 51-52 52-53 53-54 56-57 56-61 57-58 58-59
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59-60 60-61 63-64 63-68 64-65 65-66 66-67 67-68 76-77 76-81 77-78 78-79

80-81 89-90 89-94 90-91 91-92 92-93 93-94 102-103 102-107 103-104 104-105

105-106 106-107 isolated ring systems :

79-80

```
G1:Me, CH2, CH, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu
G2:NH2,[*1],[*2]
G3:[*3],[*4],[*5],[*6],[*7]
G4: [*8], [*9], [*10], [*11], [*12], [*13], [*14]
Match level :
   1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
   12:CLASS 13:CLASS 15:CLASS 16:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom
   25:Atom 26:Atom 27:CLASS 28:CLASS 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom
   37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 48:CLASS 49:Atom 50:Atom 51:Atom
   52:Atom 53:Atom 54:Atom 55:CLASS 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom
   62:CLASS 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom
   72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom
   82:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:Atom 88:Atom 89:Atom 90:Atom 91:Atom
   92:Atom 93:Atom 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 100:Atom
   102:Atom 103:Atom 104:Atom 105:Atom 106:Atom 107:Atom 108:Atom 109:Atom
   111:Atom 112:Atom 113:Atom 114:Atom 123:CLASS
Generic attributes :
   26:
   Saturation
                        : Unsaturated
   Number of Carbon Atoms : less than 7
   Type of Ring System
                      : Monocyclic
Element Count :
   Node 26: Limited
       C, C3-5
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containing 1 : 29 : 49 : 56 :

N,N1 O,O0-1 S,S0-1 =>

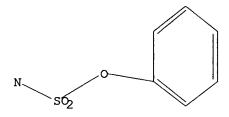
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L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam

SAMPLE SEARCH INITIATED 14:11:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 209 TO ITERATE

100.0% PROCESSED 209 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**
FED ITERATIONS: 3313 TO 50

PROJECTED ITERATIONS: 3313 TO 5047 PROJECTED ANSWERS: 2354 TO 3846

L2 50 SEA SSS SAM L1

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L3 SCREEN CREATED

=>

Uploading C:\STNEXP4\QUERIES\10019693 (patel).str

L4 STRUCTURE UPLOADED

=> que L4 NOT L3

L5 QUE L4 NOT L3

=> d 15

L5 HAS NO ANSWERS

L3 SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. L5 $$\,$ QUE $\,$ L4 NOT L3

=> s 15 sss sam

SAMPLE SEARCH INITIATED 14:14:10 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 205 TO ITERATE

100.0% PROCESSED 205 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

3241 TO 4959

PROJECTED ANSWERS: 1299 TO 2461

L6 50 SEA SSS SAM L4 NOT L3

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L7 SCREEN CREATED

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Uploading C:\STNEXP4\QUERIES\10019693 (patel).str

L8 STRUCTURE UPLOADED

=> que L8 NOT L7

L9 QUE L8 NOT L7

=> d 19

L9 HAS NO ANSWERS

L7 SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L8 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

 \Rightarrow s 19 sss sam

SAMPLE SEARCH INITIATED 14:25:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 212 TO ITERATE

100.0% PROCESSED 212 ITERATIONS

10 ANSWERS

SEARCH TIME: 00.00.01

10/019,693 (patel)

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

3367 TO 5113

PROJECTED ANSWERS:

11 TO 389

T.10

10 SEA SSS SAM L8 NOT L7

=> s 19 sss ful

FULL SEARCH INITIATED 14:26:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4126 TO ITERATE

100.0% PROCESSED 4126 ITERATIONS

255 ANSWERS

SEARCH TIME: 00.00.01

L11 255 SEA SSS FUL L8 NOT L7

. => s 111

L12

42 L11

=> d 112 1-42 bib, ab, hitstr

10/019,693 (patel)

L12 ANSWER 1 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 2003:44124 CAPLUS

DN 138:55747

ΤI Preparation of arylsulfamates as estrone sulfatase inhibitors

IN Ahmed, Sabbir

PA BTG International Limited, UK

Brit. UK Pat. Appl., 28 pp. SO CODEN: BAXXDU

DT Patent

LΑ English

FAN.CNT 1

FAN.CNI I									
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE				
		-							
PI	GB 2371299	A1	20020724	GB 2001-1220	20010117				
PRAI	GB 2001-1220		20010117						

MARPAT 138:55747 OS

AB Title compds. [I; R1-R5 = H, halo, alkyl, nitro, (substituted) alkoxy, aryl, aryloxy, alkylamino, arylamino, COOR6, sulfamate group; .gtoreq.1 of R1-R5 = sulfamate group, aryl, aryloxy, or arylamino substituted with a sulfamate group; R6 = H, aryl, or alkyl], were prepd. Thus, NaH was added to a stirred soln. of Me 4-hydroxybenzoate (prepn. given) in DMF at O.degree.; after 30 min. aminosulfonyl chloride in PhMe was added and the reaction allowed to stir for 10 h to give 31.6% Me 4-[(aminosulfonyl)oxy]benzoate. The latter inhibited estrone sulfatase by 74.7% at 50 .mu.M.

IT 319014-71-6P, Methyl 4'-[(aminosulfonyl)oxy]-1,1'-biphenyl-4carboxylate 471269-63-3P, Ethyl 4'-[(aminosulfonyl)oxy]-1,1'biphenyl-4-carboxylate 471269-64-4P, Propyl 4'-[(aminosulfonyl)oxy]-1'-biphenyl-4-carboxylate 471269-65-5P, Butyl 4'-[(aminosulfonyl)oxy]-1'-biphenyl-4-carboxylate RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(prepn. of arylsulfamates as estrone sulfatase inhibitors)

RN 319014-71-6 CAPLUS

[1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, methyl ester CN (9CI) (CA INDEX NAME)

RN 471269-63-3 CAPLUS

[1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, ethyl ester CN (9CI) (CA INDEX NAME)

RN 471269-64-4 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, propyl ester (9CI) (CA INDEX NAME)

RN 471269-65-5 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, butyl ester (9CI) (CA INDEX NAME)

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ANSWER 2 OF 42 CAPLUS COPYRIGHT 2003 ACS
L12
     2002:845557 CAPLUS
ΑN
DN
     137:353213
     Preparation of sulfamates with a steroid nucleus as steroid sulfatase
TI
     inhibitors for treating breast cancer
     Reed, Michael John; Potter, Barry Victor Lloyd
IN
PA
     Sterix Ltd., USA
     U.S., 55 pp., Cont. of U.S. Ser. No. 125,255.
SO
     CODEN: USXXAM
DT
     Patent
     English
LA
FAN.CNT 8
     PATENT NO.
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                                           APPLICATION NO.
                                                            DATE
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OS
     MARPAT 137:353213
AB
     The invention pertains to methods for introducing an estrogenic compd.
     into a subject in need thereof involving administering an effective amt.
     of a ring system compd. having the formula (I) wherein each of R1 and R2
     is independently selected from H, alkyl, alkenyl, cycloalkyl and aryl, and
     at least one of R1 and R2 is H, or together represent alkylene optionally
     contg. one or more hetero atoms or groups in the alkylene chain; and the
     ring system ABCD represents a substituted or unsubstituted, satd. or
     unsatd. steroid nucleus selected from the group consisting of estrones,
     dehydroepiandrosterones, substituted estrones, estradiols, substituted
     estradiols, estriols, substituted dehydroepiandrosterones, or substituted
     estriols; wherein the compd. is an inhibitor of an enzyme having steroid
     sulfatase activity (EC 3.1.6.2), or a pharmaceutically acceptable salt
               The compds. have application for treating breast cancer.
     243129-61-5P, Sulfamic acid, 2-methoxy-4-[[[(6E)-8-methyl-1-oxo-6-
TΥ
     nonenyl]amino]methyl]phenyl ester
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
```

(prepn. of sulfamates with a steroid nucleus as steroid sulfatase inhibitors for treating breast cancer)

RN 243129-61-5 CAPLUS

CN Sulfamic acid, 2-methoxy-4-[[[(6E)-8-methyl-1-oxo-6-nonenyl]amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

$$\begin{array}{c|c} & & & \\ &$$

RE.CNT 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/019,693 (patel)

L12 ANSWER 3 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 2002:482277 CAPLUS

DN 138:66153

The design, synthesis, and biochemical evaluation of derivatives of ΤI biphenyl sulfamate-based compounds as novel inhibitors of estrone sulfatase

Ahmed, Sabbir; James, Karen; Owen, Caroline P. ΑU

School of Chemical and Pharmaceutical Sciences, Kingston University, CS Surrey, Kingston upon Thames, KT1 2EE, UK

Biochemical and Biophysical Research Communications (2002), 294(1), \nearrow SO 180-183 CODEN: BBRCA9; ISSN: 0006-291X

PB Elsevier Science

DTJournal LА English

CASREACT 138:66153 OS

We report the initial results of our study into the use of a potential AB transition state (TS) of the reaction catalyzed by the enzyme estrone sulfatase (ES) in the design of a series of simple 4'-0-sulfamoyl-4biphenyl-based compds. as novel inhibitors of ES. The results of the study show that these compds. are: potent inhibitors, possessing greater inhibitory activity than 4-methylcoumarin-7-0-sulfamate (COUMATE); weaker inhibitors than the tricyclic deriv. of COUMATE, namely 667-COUMATE and the steroidal inhibitor estrone-3-O-sulfamate (EMATE), and irreversible inhibitors of ES.

IT 25999-01-3P

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(design, synthesis, and biochem. evaluation of derivs. of biphenyl sulfamate-based compds. as novel inhibitors of estrone sulfatase)

RN 25999-01-3 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

IT 319014-71-6P 319014-72-7P 471269-63-3P 471269-64-4P 471269-65-5P

> RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(design, synthesis, and biochem. evaluation of derivs. of biphenyl sulfamate-based compds. as novel inhibitors of estrone sulfatase)

RN 319014-71-6 CAPLUS

[1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, methyl ester CN (9CI) (CA INDEX NAME)

RN 319014-72-7 CAPLUS

CN Sulfamic acid, 4'-cyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 471269-63-3 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 471269-64-4 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, propyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & \\ \parallel & \\ H_2N-S-O & & \\ \parallel & \\ O & & O \end{array}$$

RN 471269-65-5 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, butyl ester (9CI) (CA INDEX NAME)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/019,693 (patel)

L12 ANSWER 4 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 2002:324919 CAPLUS

DN 137:310661

TI Design, synthesis and biochemical evaluation of AC ring mimics as novel inhibitors of the enzyme estrone sulfatase (ES)

AU Ahmed, Sabbir; James, Karen; Owen, Caroline P.; Patel, Chirag K.

CS School of Chemical and Pharmaceutical Sciences, Kingston University, Kingston upon Thames, Surrey, KTl 2EE, UK

SO Bioorganic & Medicinal Chemistry Letters (2002), 12(10), 1343-1346 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

AB 4-(4-RC6H4)C6H4O3SNH2 [= H, CN, CO2Me, CO2Et, CO2Pr, CO2Bu] were prepd.as novel inhibitors of the enzyme estrone sulfatase (ES). The results of the study show that these compds. are potent inhibitors, possessing greater inhibitory activity than coumate, but weaker inhibitory activity than emate or the tricyclic deriv. of coumate, namely 667-coumate.

Furthermore, the compds. are obsd. to be irreversible inhibitors.

IT 25999-01-3P 319014-71-6P 319014-72-7P 471269-63-3P 471269-64-4P 471269-65-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and estrone sulfatase inhibiting activity of sulfamoyloxybiphenyls as steroid AC ring mimics)

RN 25999-01-3 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 319014-71-6 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 319014-72-7 CAPLUS

CN Sulfamic acid, 4'-cyano[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 471269-63-3 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\ &$$

RN 471269-64-4 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, propyl ester
(9CI) (CA INDEX NAME)

RN 471269-65-5 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]-, butyl ester (9CI) (CA INDEX NAME)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 5 OF 42 CAPLUS COPYRIGHT 2003 ACS
AN
     2002:240724 CAPLUS
DN
     136:263092
TI
     Preparation of 3,4-dihydropyrroles as pesticides
     Plant, Andrew; Marhold, Albrecht; Grosser, Rolf; Erdelen, Christoph;
IN
     Turberg, Andreas; Hansen, Olaf
PA
     Bayer Aktiengesellschaft, Germany
SO
     PCT Int. Appl., 114 pp.
     CODEN: PIXXD2
DT
     Patent
     German
LA
FAN.CNT 1
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO.
                                                            DATE
PΙ
    WO 2002024644
                      A1
                            20020328
                                           WO 2001-EP10430 20010910
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
             US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                          DE 2000-10051395 20001017
                            20020411
     DE 10051395
                       A1
                                           AU 2001-87722
    AU 2001087722
                       Α5
                            20020402
                                                             20010910
PRAI DE 2000-10047119
                            20000922
                      Α
     DE 2000-10051395
                      Α
                            20001017
    WO 2001-EP10430
                       W
                            20010910
os
    MARPAT 136:263092
    Title compds. [I; n = 0, 1; r, s = 0-2; R1 = halo, Me; R2 = H, halo; R3,
AΒ
     R4 = halo, (halo)alkyl, (halo)alkoxy; R5 = (halo)alkyl, (substituted) Ph,
    NR6R7; R6 = (halo)alkyl; R7 = H, (halo)alkyl, R6R7 = (alkoxy)alkylene]
     were prepd. Thus, 4-[5-(2,6-difluorophenyl)-3,4-dihydro-2H-pyrrol-2-
     yl]phenol in PhMe was treated with 45% NaOH and 4-
     (trifluoromethoxy)benzenesulfonyl chloride, followed by stirring for 12 h
     at 45.degree., to give 70% 5-(2,6-difluorophenyl)-2-(4-[4-
     (trifluoromethoxy)phenyl]sulfonyloxyphenyl)-3,4-dihydro-2H-pyrrole.
     Several I at 100-200 ppm gave 90-95% kill of Aphis gossypii on Gossypium
    hirsutum after 6 days.
IT
     405201-75-4P
     RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN
     (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (prepn. of dihydropyrroles as pesticides)
RN
     405201-75-4 CAPLUS
     Sulfamic acid, dimethyl-, 4'-[5-(2,6-difluorophenyl)-3,4-dihydro-2H-pyrrol-
CN
```

2-yl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

IT 405201-79-8P 405201-83-4P 405201-84-5P 405201-85-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of dihydropyrroles as pesticides)

RN 405201-79-8 CAPLUS

CN Carbamic acid, [4-(2,6-difluorophenyl)-1-[4'-[[(dimethylamino)sulfonyl]oxy][1,1'-biphenyl]-4-yl]-4-oxobutyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 405201-83-4 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[4'-[[(dimethylamino)sulfonyl]oxy][1,1'-biphenyl]-4-yl]-5-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 405201-84-5 CAPLUS

CN Sulfamic acid, dimethyl-, 4'-(5-oxo-2-pyrrolidinyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 405201-85-6 CAPLUS

CN Sulfamic acid, dimethyl-, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 2002:63493 CAPLUS

DN 136:112635

Biphenylyl sulfamates as steroid sulfatase inhibitors for TΙ estrogen-dependent diseases

Jinbo, Yoshikazu; Miyasaka, Tomohiro; Inoue, Yoshimasa IN

Japan Organo Co., Ltd., Japan PA

Jpn. Kokai Tokkyo Koho, 14 pp. SO CODEN: JKXXAF

DTPatent

Japanese LΑ

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE 20000706 PΙ JP 2002020362 A2 20020123 JP 2000-245314 20000706

PRAI JP 2000-245314

os MARPAT 136:112635

4-RC6H4C6H4OSO2NH2-4 [I; R = CO2H, CONR1R2, CONR1OCH2Ph, COR2, C(OH)R1R2; AB R1 = H, (un) substituted alkyl; 2 = (un) substituted alkyl] are prepd. I are useful for treatment of mammary cancer, endometrial cancer, endometriosis, uterine myoma, etc. I (R = COCH2C6H4CMe3-4) (prepn. given) inhibited human placenta-derived steroid sulfatase at IC50 3.6 .mu.M.

IT 390358-08-4P 390358-09-5P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

> (prepn. of biphenylyl sulfamates as steroid sulfatase inhibitors for treatment of estrogen-dependent diseases)

390358-08-4 CAPLUS RN

Sulfamic acid, 4'-acetyl[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME) CN

RN 390358-09-5 CAPLUS

CN Sulfamic acid, 4'-[[4-(1,1-dimethylethyl)phenyl]acetyl][1,1'-biphenyl]-4yl ester (9CI) (CA INDEX NAME)

$$H_2N-S-O$$
 $C-CH_2$
 $Bu-t$

IT 390358-11-9P 390358-12-0P 390358-14-2P 390358-16-4P 390358-17-5P 390358-19-7P 390358-21-1P 390358-23-3P 390358-25-5P 390358-27-7P 390358-29-9P 390358-31-3P 390358-33-5P 390358-34-6P 390358-35-7P

390358-36-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of biphenylyl sulfamates as steroid sulfatase inhibitors for treatment of estrogen-dependent diseases)

RN 390358-11-9 CAPLUS

CN Sulfamic acid, 4'-(1-oxopentyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ H_2N-S-O & & & \\ & & & \\ & & & \\ O & & & \\ \end{array}$$

RN 390358-12-0 CAPLUS

CN Sulfamic acid, 4'-(1-oxoheptyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 390358-14-2 CAPLUS

CN Sulfamic acid, 4'-[(ethylamino)carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 390358-16-4 CAPLUS

CN Sulfamic acid, 4'-[(octylamino)carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

Me- (CH₂)
$$_{7}$$
-NH-C

O

O

S
NH₂

O

O

RN 390358-17-5 CAPLUS

CN Sulfamic acid, 4'-[[(2-phenylethyl)amino]carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 390358-19-7 CAPLUS

CN Sulfamic acid, 4'-[[[[4-(1,1-dimethylethyl)phenyl]methyl]amino]carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & & \\ H_2N-S-O & & & & \\ & & & \\ O & & & \\ \end{array}$$

RN 390358-21-1 CAPLUS

CN Sulfamic acid, 4'-[[[4-(1,1-dimethylethyl)phenyl]amino]carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O & O \\ H_2N-S-O & 0 \\ O & C-NH \end{array}$$

RN 390358-23-3 CAPLUS

CN Sulfamic acid, 4'-[[(phenylmethoxy)amino]carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 390358-25-5 CAPLUS

CN Sulfamic acid, 4'-[[methyl(phenylmethyl)amino]carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 390358-27-7 CAPLUS

CN Sulfamic acid, 4'-[[[[4-(1,1-dimethylethyl)phenyl]methyl]methylamino]carbo nyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & Me \\ H_2N-S-O & Me \\ C-N-CH_2 & \\ \end{array}$$

RN 390358-29-9 CAPLUS

CN Sulfamic acid, 4'-[[butyl(phenylmethyl)amino]carbonyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ H_2N-S-O & & & C-N-Bu-n \\ \parallel & & \parallel & \parallel \\ O & & & O & CH_2-Ph \end{array}$$

RN 390358-31-3 CAPLUS

CN Sulfamic acid, 4'-[[[[4-(1,1-dimethylethyl)phenyl]methyl]octylamino]carbon yl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 390358-33-5 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(aminosulfonyl)oxy]- (9CI) (CA INDEX NAME)

RN 390358-34-6 CAPLUS

CN Sulfamic acid, 4'-(1-hydroxyethyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 390358-35-7 CAPLUS

CN Sulfamic acid, 4'-[2-[4-(1,1-dimethylethyl)phenyl]-1-hydroxyethyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 390358-36-8 CAPLUS

CN Sulfamic acid, 4'-[2-[4-(1,1-dimethylethyl)phenyl]-1-hydroxy-1-methylethyl][1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & Me \\ H_2N-S-O & C-CH_2 \\ O & OH \\ \end{array}$$

- L12 ANSWER 7 OF 42 CAPLUS COPYRIGHT 2003 ACS
- AN 2001:668347 CAPLUS
- DN 135:226790
- TI Preparation of aryl sulfamates for the treatment of estrogen-dependent illnesses
- IN Li, Pui-kai; Selcer, Kyle W.
- PA Duquesne University of the Holy Ghost, USA
- SO U.S., 15 pp., Cont.-in-part of U.S. Ser. No. 164,889. CODEN: USXXAM
- DT Patent
- LA English
- FAN.CNT 2

TAV. CN1 Z									
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE				
		-							
ΡI	US 6288107	В1	20010911	US 2000-536331	20000324				
	US 6248780	В1	20010619	US 1998-164889	19981001				
	US 6433000	В1	20020813	US 2001-845850	20010430				
	US 2003008862	A1	20030109	US 2002-174092	20020618				
PRAI	US 1998-164889	A2	19981001						
	US 2000-536331	A 3	20000324 .						
	US 2001-845850	A3	20010430						
		_							

- OS MARPAT 135:226790
- AΒ Sulfatase inhibitor/estrogen receptor blocker compds. (I) [wherein R = estrogen receptor blocker; R1 and R2 = independently H or alkyl] useful in the treatment of estrogen-dependent illnesses, such as breast cancer, vaginal cancer, endometrial cancer, ovarian cancer, and endometriosis, are disclosed. Prepn. and testing of 7,8-dihydro-5,6-diphenylnaphthalen-2-yl sulfamates and (Z)-4-hydroxytamoxifen sulfamate are described, and 3-benzoyl-2-phenylbenzothiophen-6-yl sulfamates (no prepn.) are claimed. Thus, 1-bromo-4-[2-(tributylsiloxy)ethoxy]benzene was treated with BuLi and then coupled with 6-(tetrahydropyranyloxy)tetralone (prepn. of reactants given) to afford the protected dihydronaphthalene (65.7%). Deprotection and bromination using pyridinium tribromide (90.3%), followed by arylation with PhLi (94%), iodination (95%), amination with NHMe2 $\,$ (88.3%), and reaction with sulfamoyl chloride (91.6%), gave II. In a sulfatase activity assay, II inhibited estrone sulfatase in rat liver microsomes at 20 .mu.M substrate estrone sulfate by over 60% compared to the control.

IT 221214-41-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of aryl sulfamates for treatment of estrogen-dependent illnesses)

- RN 221214-41-1 CAPLUS
- CN Sulfamic acid, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]phenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 8 OF 42 CAPLUS COPYRIGHT 2003 ACS
AN
     2001:338504 CAPLUS
ĎΝ
     134:340518
     Substituted 5-benzyl-2,4-diaminopyrimidines
TI
    Guerry, Philippe; Mohr, Peter; Muller, Marc; Mueller, Werner; Pflieger,
IN
     Philippe
     F. Hoffmann-La Roche A.-G., Switz.
PA
SO
     PCT Int. Appl., 177 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     German
FAN.CNT 1
     PATENT NO.
                     KIND DATE
                                          APPLICATION NO.
                                                            DATE
     WO 2001032633
                            20010510
                                          WO 2000-CH575
                                                            20001027
PΙ
                      A1
        W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ,
             DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,
             JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG,
             MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,
             TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG,
            KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                          20020814
                                           EP 2000-969149 20001027
     EP 1230224
                      A1
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL
PRAI CH 1999-2021
                      Α
                            19991104
     WO 2000-CH575
                       W
                            20001027
os
     MARPAT 134:340518
     Substituted 5-benzyl-2,4-diaminopyrimidines I [R1 = C2-C3 alkyl; R2 =
AΒ
     (un) substituted heterocyclyl, Ph, naphthyl; R3 = (un) substituted alkyl,
     alkenyl, cycloalkyl, cycloalkylalkyl, heterocyclylalkyl, alkylsulfonyl,
     cycloalkylsulfonyl, cycloalkylalkylsulfamoyl, heterocyclylsulfonyl,
     heterocyclyalkylsulfonyl, dialkylsulfamoyl] were prepd. for use as
     antibacterial agents. Thus, I [R1 = R3 = Et, R2 = I] was prepd. from
     3,5-(HO)2C6H3CO2H by iodination, esterification, etherification, redn. to
     4,3,5-I(EtO)2C6H2CHO via 4,3,5-I(EtO)2C6H2CH2OH, reaction with
     PhNHCH2CH2CN, and cyclization with guanidine-HCl. I [R1 = R3 = Et, R2 =
     I] was coupled with 3-H2NC6H4B(OH)2 to give I [R1 = R3 = Et, R2 =
     3-H2NC6H4] which had an IC50 against dihydrofolate reductase from
     Streptococcus pneumoniae 1/1 of 0.19 .mu.M.
IT
     338456-51-2P 338457-64-0P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
        (prepn. of substituted 5-benzyl-2,4-diaminopyrimidines as bacterial
        dihydrofolate reductase inhibitors)
RN
     338456-51-2 CAPLUS
     Sulfamic acid, dimethyl-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-
CN
     4'-hydroxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)
```

$$\begin{array}{c|c}
O & NH_2 \\
Me_2N-S & O \\
O & NH_2
\end{array}$$

$$NH_2 \\
NH_2$$

$$NH_2$$

RN 338457-64-0 CAPLUS

CN Sulfamic acid, dimethyl-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'-(methylthio)[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

TT 338456-43-2P 338456-46-5P 338456-48-7P 338456-50-1P 338456-55-6P 338456-57-8P 338456-58-9P 338456-60-3P 338456-61-4P 338456-65-8P 338456-71-6P 338456-72-7P 338456-76-1P 338456-79-4P 338456-87-4P 338456-82-9P 338456-83-0P 338456-92-1P 338456-94-3P 338456-95-4P 338457-65-1P 338457-66-2P 338457-97-98-0P 338458-02-9P 338458-06-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of substituted 5-benzyl-2,4-diaminopyrimidines as bacterial dihydrofolate reductase inhibitors)

RN 338456-43-2 CAPLUS

CN Sulfamic acid, dimethyl-, 3'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

RN 338456-46-5 CAPLUS

CN Sulfamic acid, methyl(1-methylethyl)-, 3'-amino-4-{(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

RN 338456-48-7 CAPLUS

CN Sulfamic acid, ethylmethyl-, 3'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

RN 338456-50-1 CAPLUS

CN Sulfamic acid, diethyl-, 3'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

RN 338456-55-6 CAPLUS

CN Sulfamic acid, methyl(1-methylethyl)-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'-hydroxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

HO OET
$$CH_2$$
 N NH_2 $i-Pr-N-S-O$ $Me O$

RN 338456-57-8 CAPLUS

CN Sulfamic acid, ethylmethyl-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'-hydroxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

HO OET
$$CH_2$$
 N NH_2 NH_2

RN 338456-58-9 CAPLUS

CN Sulfamic acid, diethyl-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'-hydroxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

HO OET
$$CH_2$$
 NH_2 NH_2 NH_2 NH_2 NH_2 NH_2 NH_2 NH_2 NH_2

RN 338456-59-0 CAPLUS

CN Sulfamic acid, dimethyl-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'-methoxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

RN 338456-60-3 CAPLUS

CN Sulfamic acid, dimethyl-, 4'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & NH_2 \\ Me_2N - S & O \\ O & NH_2 \\ N & NH_2$$

RN 338456-61-4 CAPLUS

CN Sulfamic acid, ethylmethyl-, 4'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

RN 338456-65-8 CAPLUS

CN Sulfamic acid, diethyl-, 4'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OEt} & \text{NH2} \\ \text{H2N} & \text{CH2} & \text{N} \\ \text{Et2N-S-O} & \text{NH2} \\ \text{O} & \text{OPT} & \text{NH2} \\ \text{OPT} & \text{OPT} & \text{NH2} \\ \text{OPT} & \text{OPT} & \text{OPT} & \text{OPT} \\ \text{OPT} & \text{OPT} \\ \text{OPT} & \text{OPT} & \text{OPT} \\ \text{$$

RN 338456-71-6 CAPLUS

CN Sulfamic acid, dimethyl-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'-(methylamino)[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

RN 338456-72-7 CAPLUS

CN Sulfamic acid, ethylmethyl-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6ethoxy-4'-(methylamino)[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

RN 338456-76-1 CAPLUS

CN Sulfamic acid, diethyl-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'- (methylamino)[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & NH_2 \\ Et_2N - S & O \\ \hline O & NH_2 \\ \hline N & NH_2 \\ \hline MeNH & OEt \\ \end{array}$$

RN 338456-79-4 CAPLUS

CN Sulfamic acid, dimethyl-, 4'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-3'-methyl[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & O & Me \\ & Me_2N-S & O & NH_2 \\ \hline & NH_2 & O & \\ & & OEt \\ \hline & H_2N & N & \\ \end{array}$$

RN 338456-80-7 CAPLUS

CN Sulfamic acid, ethylmethyl-, 4'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-3'-methyl[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

RN 338456-82-9 CAPLUS

CN Sulfamic acid, dimethyl-, 4'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-3'-fluoro[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Me}_2\text{N} - & & \\ & & \\ \text{NH}_2 & & \\ & & \\ \text{OEt} & & \\ & & \\ \text{NH}_2 & & \\ & & \\ \text{OEt} & & \\ \end{array}$$

RN 338456-83-0 CAPLUS

CN Sulfamic acid, ethylmethyl-, 4'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-3'-fluoro[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

RN 338456-87-4 CAPLUS

CN Sulfamic acid, dimethyl-, 3'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-5'-fluoro[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Me}_2\text{N} - & \\ & & \\ \text{N} & \\ & & \\ & & \\ \text{NH}_2 & \\ \end{array}$$

RN 338456-88-5 CAPLUS

CN Sulfamic acid, ethylmethyl-, 3'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-5'-fluoro[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

RN 338456-90-9 CAPLUS

CN Sulfamic acid, dimethyl-, 3'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'-(4-morpholinylmethyl)[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 338456-92-1 CAPLUS

CN Sulfamic acid, ethylmethyl-, 3'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'-(4-morpholinylmethyl)[1,1'-biphenyl]-2-ylester (9CI) (CA INDEX NAME)

RN 338456-94-3 CAPLUS

CN Sulfamic acid, dimethyl-, 3'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'-methyl[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & \\ & & & & \\ \text{Me}_2\text{N} - & & & \\ & & & \\ & & & \\ \text{NH}_2 & & & \\ & & & \\ \text{OEt} & & & \\ & & & \\ & & & \\ \text{NH}_2 & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\$$

RN 338456-95-4 CAPLUS

CN Sulfamic acid, ethylmethyl-, 3'-amino-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'-methyl[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

RN 338457-65-1 CAPLUS

CN Sulfamic acid, dimethyl-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & NH_2 \\ Me_2N-S-O & CH_2 \\ O & NH_2 \\ \end{array}$$

RN 338457-66-2 CAPLUS

CN Sulfamic acid, dimethyl-, 4'-amino-3'-cyano-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Me}_2\text{N} - \text{S} & & \\ & & & \\ \text{NH}_2 & & \\ & & & \\ \text{NH}_2 & & \\ & & & \\ \text{OEt} & & \\ \end{array}$$

RN 338457-67-3 CAPLUS

CN Sulfamic acid, dimethyl-, 5-[(2,4-diamino-5-pyrimidinyl)methyl]-3-ethoxy-2-(1H-indol-5-yl)phenyl ester (9CI) (CA INDEX NAME)

$$NH_2$$
 $O-S-NMe_2$
 $O-S-NMe_2$

RN 338457-92-4 CAPLUS

CN Sulfamic acid, dimethyl-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'-(methylsulfonyl)[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O & NH2 \\
 & NH2 & NH2 \\
 & O & NH2 \\
 & NH2 & NH2 \\
 & NH2 & NH2 \\
 & NH2 & NH2 \\
 & O & NH2 & NH2 \\
 & O & O & O & O & O \\
 & O & O & O & O & O \\
 & O & O & O & O & O & O \\
 & O & O & O & O & O & O \\
 & O & O & O & O & O & O \\
 & O & O & O & O & O & O \\
 & O & O & O & O & O & O \\
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 & O & O & O & O & O \\
 & O & O & O & O & O \\
 & O & O & O & O & O \\
 & O &$$

RN 338457-95-7 CAPLUS

CN Sulfamic acid, dimethyl-, 4'-(acetyloxy)-4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O & NH_2 \\
Me_2N - S & O \\
O & NH_2
\end{array}$$

$$AcO & OEt$$

RN 338457-98-0 CAPLUS

CN Sulfamic acid, dimethyl-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-3'-fluoro-4'-(4-morpholinylmethyl)[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 338458-02-9 CAPLUS

CN Sulfamic acid, dimethyl-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'-(4-morpholinylmethyl)[1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Me}_2\text{N} - \text{S} & \text{O} \\ & & & \\ \text{H}_2\text{N} & & & \\ & & & \\ \text{N} & & & \\ & & & \\ \text{N} & & & \\ & & & \\ \text{N} & & \\ \end{array}$$

RN 338458-06-3 CAPLUS

CN Sulfamic acid, dimethyl-, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6-ethoxy-4'-[[(2-fluoroethyl)methylamino]methyl][1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 10 OF 42 CAPLUS COPYRIGHT 2003 ACS
L12
     2000:875743 CAPLUS
AN
     134:29611
DN
     Preparation of O-sulfamoylphenols for pharmaceutical use as steroid
ΤI
     sulfatase inhibitors
     Reed, Michael John; Potter, Barry Victor Lloyd
IN
     Sterix Limited, UK
PA
     U.S., 56 pp., Cont.-in-part of U.S. 6,011,024.
SO
     CODEN: USXXAM
DT
     Patent
     English
LΑ
FAN.CNT 8
                            DATE
                                            APPLICATION NO.
                                                              DATE
     PATENT NO.
                      KIND
     US 6159960
                       Α
                             20001212
                                            US 1998-193969
                                                              19981118
    <u>EP 9211</u>30
                                            EP 1998-204340
                                                              19920828
                       A2
                             19990609
     EP 921130
                       Ā3
                            20010905
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE
                            19990714
                                            EP 1998-204337
                                                              19920828
     EP 928609
                       A2
     EP 928609
                       A3
                            20011107
     EP 928609
                       В1
                            20030416
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE
                                            JP 1999-211413
                       A2
                                                              19920828
     JP 2000038341
                            20000208
     EP 982032
                                            EP 1999-203449
                                                              19920828
                       A2
                            20000301
                       A3 ′
     EP 982032
                            20020320
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE
                                            JP 2000-163410
                                                              19920828
                       A2
                            20001226
     JP 2000355542
                       №2
                                            JP 2000-163411
                                                              19920828 -
     JP 2000355598
                             20001226
                                            EP 2000-204525
     EP 1099706
                       A2
                             20010516
                                                              19920828
     EP 1099706
                       A3
                             20020904
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE
         R:
     JP 2002255993
                       A2
                             20020911
                                            JP 2002-17765
                                                              19920828
                             19981103
                                            US 1995-458352
                                                              19950602
     US 5830886
                       Α
                             20000104
                                            US 1998-111927
                                                              19980708
     US 6011024
                       Α
     AU 9910077
                       A1
                            19990304
                                            AU 1999-10077
                                                              19990111
     AU 717116
                       B2
                            20000316
                                            AU 2000-10130
                                                              20000106
     AU 726811
                       B2
                            20001123
                            19910829
PRAI GB 1991-18478
                       Α
                            19950602
     US 1995-458352
                       A2
                       A2
                            19980708
     US 1998-111927
                       Α3
                            19920828
     EP 1992-918285
     EP 1998-204340
                       A3
                            19920828
                       Α3
                            19920828
     JP 1993-505032
     JP 2000-163410
                       A3
                            19920828
     US 1994-196192
                       Α3
                            19941227
    WO 1997-GB444
                       A2
                            199702I7
     WO 1997-GB600
                       A2
                             19970304
     WO 1997-GB3352
                       A2
                             19971204
                       A3
                             19980618
     AU 1998-71952
     AU 1999-10077
                       Α
                             19990111
OS
     MARPAT 134:29611
     O-sulfamoylphenols, R1R2N-SO2-OR [R = aryl bonded through a benzene
AB
     subunit, such as Ph, estra-1,3,5(10)-trien-3-yl, coumarinyl, flavonyl,
     flavanyl, isoflavonyl; R1, R2 = H, alkyl, alkenyl, cycloalkyl, aryl], were
     prepd. for use as steroid sulfatase inhibitors for the treatment of
```

diseases, such as breast cancer. Thus, osterone was reacted with sulfamoyl chloride using NaH in DMF to give sulfamate I. The prepd. sulfamates were tested for inhibiting activity against steroid sulfatase

enzyme (E.C.3.1.6.2).

IT 243129-61-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of O-sulfamoylphenols for pharmaceutical use as steroid sulfatase inhibitors)

RN 243129-61-5 CAPLUS

CN Sulfamic acid, 2-methoxy-4-[[[(6E)-8-methyl-1-oxo-6-nonenyl]amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

$$\begin{array}{c|c}
\text{MeO} & \\
\text{O} & \text{O} \\
\text{H}_2\text{N} & \text{S}_0
\end{array}$$

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 11 OF 42 CAPLUS COPYRIGHT 2003 ACS
AN
     2000:227501 CAPLUS
DN
     132:260691
    Aromatic sulfamate derivative sulfatase inhibitor/estrogen receptor
ΤI
    blocker compounds for the treatment of estrogen-dependent illnesses, and
    methods for preparation and use
     Li, Pui-Kai; Selcer, Kyle W.
IN
     Duquesne University of the Holy Ghost, USA
PA
SO
     PCT Int. Appl., 28 pp.
     CODEN: PIXXD2
     Patent
DT
     English
LA
FAN.CNT 2
                      KIND DATE
     PATENT NO.
                                           APPLICATION NO.
                                                            DATE
                            _____
                      ____
                                           WO 1999-US22823 19990930
                            20000406
    WO 2000018397
                      A1
         W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
             CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD,
             MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK,
             SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                            20010619
                                           US 1998-164889
                                                            19981001
     US 6248780
                       В1
                            20000406
                                           CA 1999-2345988
                                                            19990930
     CA 2345988
                       AΑ
                            20000417
                                           AU-1999-64081
                                                            19990930
    AU 9964081
                       Α1
     AU 748958
                       В2
                            20020613
                                           EP 1999-951694
                                                            19990930
     EP 1117395
                       A1
                            20010725
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
                       Т2
                            20020813
                                           JP 2000-571915
                                                            19990930
     JP 2002525322
PRAI US 1998-164889
                       Α
                            19981001
     WO 1999-US22823
                       W
                            19990930
os
    MARPAT 132:260691
AΒ
     Sulfatase inhibitor/estrogen receptor blocker compds. useful in the
     treatment of estrogen dependent illnesses are disclosed. The compds.
     generally comprise a sulfamate moiety and an arom., estrogen receptor
     blocker moiety. Methods for synthesizing these compds. and using them in
     the therapeutic and/or prophylactic treatment of an estrogen-dependent
     disease are also disclosed. Prepn. and testing of (Z)-4-hydroxytamoxifen
     sulfamate is described.
IT
     221214-42-2P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (arom. sulfamate deriv. sulfatase inhibitor/estrogen receptor blocker
        compds. for the treatment of estrogen-dependent illnesses, and methods
        for prepn. and use)
RN
     221214-42-2 CAPLUS
     Sulfamic acid, 4-[(12)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-
CN
     butenyl]phenyl ester (9CI) (CA INDEX NAME)
```

Double bond geometry as shown.

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 12 OF 42 CAPLUS COPYRIGHT 2003 ACS
AN
     2000:190770 CAPLUS
DN
     132:222555
     Preparation of interleukin-5 inhibiting 6-azauracil derivatives
ΤI
     Freyne, Eddy Jean Edgard; Lacrampe, Jean Fernand Armand; Deroose, Frederik
IN
     Dirk; Venet, Marc Gaston
     Janssen Pharmaceutica N.V., Belg.
PΑ
SO
     Eur. Pat. Appl., 37 pp.
     CODEN: EPXXDW
DT
     Patent
     English
LΑ
FAN.CNT 1
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO.
                                                             DATE
                                           ______
                            20000322
                                                             19980918
                                           EP 1998-203148
PΙ
     EP 987265
                      A1
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
                                           CA 1999-2344390 19990914
     CA 2344390
                       AΑ
                            20000330
     WO 2000017195
                       A1
                            20000330
                                           WO 1999-EP6776
                                                            19990914
            AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
             CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD,
             MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK,
             SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                            20000410
                                          AU 1999-60825
                                                             19990914
     AU 9960825
                       A1
                                           EP 1999-947336
                                                            19990914
     EP 1114046
                       A1
                            20010711
     EP 1114046
                       В1
                            20030423
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
                            20020820
                                           JP 2000-574104
                                                             19990914
     JP 2002526495
                       Т2
     US 2002010177
                       A1
                            20020124
                                           US 2001-812731
                                                             20010319
PRAI EP 1998-203148
                       Α
                            19980918
     WO 1999-EP6776
                       W
                            19990914
     MARPAT 132:222555
OS
     The title compds. [I; p = 0-4; X = 0, S, NR5, a direct bond; Y = 0, S,
AB
     NR5, SO2; R1 = alkyl, halo, polyhaloalkyl, etc.; R2 = Het1, cycloalkyl,
     alkyl, and if X = O, S, NR5, then R2 may also represent aminocarbonyl,
     aminothiocarbonyl, alkylcarbonyl, etc.; R3, R4 = H, alkyl, cycloalkyl;
     R3R4 = alkanediyl; R5 = H, alkyl; Het1 = (un)substituted heterocycle],
     useful for treating eosinophil-dependent inflammatory diseases, and
     marking a receptor, were prepd. and formulated. E.g., a multi-step
     synthesis of 1,2,4-triazine-3,5(2H,4H)-dione II which showed 90.5%
     inhibition of IL-5 prodn., was given.
IT
     261512-01-0P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of interleukin-5 inhibiting 6-azauracil derivs.)
RN
     261512-01-0 CAPLUS
     Sulfamic acid, 3-[2-[1-[2,6-dichloro-4-(4,5-dihydro-3,5-dioxo-1,2,4-
CN
     triazin-2(3H)-yl)phenyl]-1-methylethyl]-4-phenyl-5-thiazolyl]phenyl ester
           (CA INDEX NAME)
```

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 13 OF 42 CAPLUS COPYRIGHT 2003 ACS
AN
     2000:84826 CAPLUS
DN
     132:137416
     Preparation of 6-[[[[phosphono(oxy)]aryl]alkanoyl]amino]-1,4-thiazepin-5-
TI
     ones and analogs as protein tyrosine kinase c-Src inhibitors
     Benard, Didier; Deprez, Pierre; Lesuisse, Dominique; Mandine, Eliane;
IN
     Ugolini, Antonio
PA
     Hoechst Marion Roussel, Fr.
     PCT Int. Appl., 151 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     French
LA
FAN.CNT 1
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO.
                                                            DATE
                                           _____
                            20000203
                                          WO 1999-FR1770
                                                            19990720
PΙ
     WO 2000005246
                      A1
        W: AE, AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GD, GE, HR, HU,
             ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX,
             NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, ZA, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,
             ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,
             CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                           FR 1998-9258
     FR 2781483
                      A1
                            20000128
                                                            19980721
     AU 9949133
                            20000214
                                           AU 1999-49133
                                                            19990720
                       A1
PRAI FR 1998-9258
                       Α
                            19980721
     WO 1999-FR1770
                            19990720
                       W
OS - MARPAT 132:137416
     Title compds. [I; R = NHZZ1Z2R7; R1,R2 = H, OH, alkyl, alkoxy, etc.; R1R2
ΑB
     = atoms to complete a (hetero)arom. ring; R3,R4 = H, alkyl, aryl(alkyl),
     etc.; R5 = H, alk(en)yl, aryl(alkyl), etc.; R7 = P(O)(OH)2, OP(O)(OH)2,
     bis(alkoxy)phosphoryl(oxy), CH2CO2H, SO2NH2, etc.; Z = CO, SO2,
     alk(en)ylene, etc.; Z1 = CHR6(CH2)1-4, CR6:CHCH2, CHR6, etc.; R6 = H,
     (acyl)amino, tetrazolyl, etc.; Z2 = arylene; dashed line = optional addnl.
     bond] were prepd. Thus, (S)-HSCH2CH(NH2)CO2Me was cyclocondensed with
     CLCH2CH2NH2 and the product amidated by (S)-HO2CCH(NHBoc)CH2C6H4[OP(O)(OCH
     2Ph(2)-4 to give, in 2 addnl. steps, [S-[R*(6S*)]]-I [R =
     NHCOCH (NHBoc) CH2C6H4 [OP (O) (OCH2Ph)2]-4, R1-R4 = H, R5 =
     3-cyclohexylpropyl, dashed line = null]. Data for biol. activity of I
     were given.
IT
     256655-91-1P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of 6-[[[phosphono(oxy)]aryl]alkanoyl]amino]-1,4-thiazepin-5-
        ones and analogs as protein tyrosine kinase c-Src inhibitors)
RN
     256655-91-1 CAPLUS
     Sulfamic acid, 4-[[(6R)-hexahydro-5-oxo-4-(3-phenyl-2-propenyl)-1,4-
CN
     thiazepin-6-yl]amino]carbonyl]phenyl ester- (9CI) (CA INDEX NAME)
```

Absolute stereochemistry.

Double bond geometry unknown.

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 14 OF 42 CAPLUS COPYRIGHT 2003 ACS
AN
     2000:10623 CAPLUS
DN
     132:78747
     Preparation and formulation of steroid sulphatase inhibitors for use in
ΤI
     cancer treatment
     Reed, Michael John; Potter, Barry Victor Lloyd
IN
     Imperial College of Science Technology and Medicine, UK
PA
     U.S., 56 pp., Cont.-in-part of U.S. 5,830,886.
SO
     CODEN: USXXAM
DT
     Patent
     English
LА
FAN.CNT 8
     PATENT NO.
                       KIND DATE
                                              APPLICATION NO.
                                                                DATE
                             ----<del>-</del>
                              20000104
                                                                19980708
                                              US 1998-111927
PΙ
     US 6011024
                        Α
                              19990609
                                              EP 1998-204340
                                                                19920828
                        A2
     EP 921130
                              20010905
     EP 921130
                        A3
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE
     EP 928609
                        A2
                              19990714
                                             EP 1998-204337
                                                                19920828
     EP 928609
                        A3
                              20011107
     EP 928609
                        В1
                              20030416
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE
                              20000208
                                              JP 1999-211413
                                                                19920828
     JP 2000038341
                        A2
     EP 982032
                              20000301
                                              EP 1999-203449
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     EP 982032
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                        Α3
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                        A2
                              20001226
                                              JP 2000-163410
                                                                19920828
     JP 2000355542
                                              JP 2000-163411
     JP 2000355598
                        A2
                              20001226
                                                                19920828
                                              EP 2000-204525
                              20010516
                                                                19920828
     EP 1099706
                        A2
                              20020904
     EP 1099706
                        Α3
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE
                             20020911
                                              JP 2002-17765
                                                                19920828
     JP 2002255993
                        A2
                                              US 1994-196192
     US 5616574
                        Α
                              19970401
                                                                19941227
     US 5830886
                              19981103
                                              US 1995-458352
                                                                19950602
                        Α
     WO 9730041
                        Α1
                              19970821
                                              WO 1997-GB444
                                                                19970217
             AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT,
              RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN,
              AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,
              IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML,
              MR, NE, SN, TD, TG
                                              WO 1997-GB600
                              19970912
                                                                19970304
     WO 9732872
                        A1
             AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CU, CZ, DE, DK,
              EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC,
              LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT,
              RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN,
              YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
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             ML, MR, NE, SN, TD, TG
                        A2
                              19980611
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              KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ,
              PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG,
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US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR,
             GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA,
             GN, ML, MR, NE, SN, TD, TG
                                            US 1998-193969
                                                              19981118
     US 6159960
                       Α
                            20001212
                                            US 1998-193970
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                            20021105
     US 6476011
                       В1
                                            AU 1999-10077
                                                              19990111
     AU 9910077
                       A1
                            19990304
     AU 717116
                       B2
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                       В1
                                            US 1999-238345
                                                              19990127
     US 6187766
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     AU 726811
                       B2
                            20001123
                                            AU 2000-10130
                                                              20000106
                       В1
                            20030114
                                            US 2000-638315
                                                              20000814
     US 6506792
     US 2001018435
                       A1
                            20010830
                                            US 2001-794853
                                                             20010227
     US 2002177619
                       A1
                            20021128
                                            US 2002-82007
                                                              20020221
     US 2002128243
                       A1
                            20020912
                                            US 2002-84235
                                                             20020225
PRAI GB 1991-18478
                       Α
                            19910829
     US 1994-196192
                       A3
                            19941227
     US 1995-458352
                       A2
                            19950602
                       A2
                            19970217
    WO 1997-GB444
     WO 1997-GB600
                       A2
                            19970304
     WO 1997-GB3352
                       A2
                            19971204
     EP 1992-918285
                       A3
                            19920828
     EP 1998-204340
                       A3
                            19920828
     JP 1993-505032
                            19920828
                       Α3
     JP 2000-163410
                            19920828
                       А3
                       W
     WO 1992-GB1587
                            19920828
     GB 1996-3325
                            19960216
                       Α
     GB 1996-4709
                       Α
                            19960305
     GB 1996-5725
                       Α
                            19960319
     GB 1996-25334
                       Α
                            19961205
     AU 1998-71952
                       А3
                            19980618
                       A2
                            19980708
     US 1998-111927
                       A2
                            19980814
     US 1998-125255
     US 1998-142194
                       A2
                            19980902
     US 1998-193970
                       Α3
                            19981118
     AU 1999-10077
                            19990111
                       Α
     US 1999-238345
                       A2
                            19990127
     US 2000-579163
                       Α3
                            20000525
OS
     MARPAT 132:78747
     Steroid sulfatase inhibitors, R1R2NSO2OR [R = arom. ring, such as Ph,
ΑB
     estra-1,3,5(10)-trien-3-yl, coumarinyl, flavonoid; R1, R2 = H, alkyl,
     alkenyl, cycloalkyl, aryl; R1R2 = alkylene], were prepd. for use in the
     treatment of estrogen dependent tumors. Thus, sulfamate I was prepd. by
     sulfamoylation of oestrone with sulfamoyl chloride. The prepd. compds.
     were tested for steroid sulfatase enzyme, E.C. 3.1.6.2, and aromatase
     inhibiting activity.
IT
     243129-61-5P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. and formulation of steroid sulfatase inhibitors for use in
        treatment of cancer)
RN
     243129-61-5
                 CAPLUS
     Sulfamic acid, 2-methoxy-4-[[[(6E)-8-methyl-1-oxo-6-
CN
```

Double bond geometry as shown.

nonenyl]amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
\text{MeO} & \\
\text{O} & \\
\text{O} & \\
\text{H}_2\text{N} & \\
\end{array} \begin{array}{c}
\text{CH}_2\text{)}_{4} & \\
\text{E} & \\
\text{Pr-i} & \\
\end{array}$$

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L12 ANSWER 15 OF 42 CAPLUS COPYRIGHT 2003 ACS
- AN 1999:437570 CAPLUS
- DN 131:208593
- TI Recent advances in the development of steroid sulfatase inhibitors
- AU Purohit, A.; Hejaz, H. A. M.; Woo, L. W. L.; Van Strien, A. E.; Potter, B. V. L.; Reed, M. J.
- CS Endocrinology and Metabolic Medicine, Imperial College School of Medicine, St Mary's Hospital, London, W2 1NY, UK
- Journal of Steroid Biochemistry and Molecular Biology (1999), 69(1-6), 227-238
 - CODEN: JSBBEZ; ISSN: 0960-0760 Elsevier Science Ltd.
- PB Elsevier
 DT Journal
- LA English
- Inhibition of steroid sulfatase is now an important target for the AB development of new drugs for the treatment of women with endocrine-dependent breast tumors. The first potent sulfatase inhibitor identified, estrone-3-O-sulfamate (EMATE) proved, unexpectedly, to be estrogenic. A no. of strategies have therefore been adopted to design and synthesize a nonoestrogenic inhibitor. For this, a no. of modifications have been made to the A and D rings of the estrone nucleus. Methoxyestrone-3-O-sulfamate, while having similar in vitro and in vivo sulfatase inhibitory potency to that of EMATE, was devoid of estrogenic activity when tested at 2 mg/kg in an ovariectomized rat uterine wt. gain assay. 17-Deoxyestrone-3-O-sulfamate was also a potent steroid sulfatase inhibitor and while it was devoid of estrogenic activity when tested at 0.1 mg/kg, did stimulate uterine growth at 1.0 mg/kg. As an alternative approach to the use of steroid-based inhibitors a no. of single ring, bicyclic non-fused ring, and two fused ring sulfamate analogs were designed, synthesized and tested for their ability to inhibit steroid sulfatase activity. In general, although the single ring and bicyclic non-fused ring sulfamate analogs could inhibit sulfatase activity, they were considerably less potent than EMATE. The mono- and bis-sulfamate derivs. of 5,7-dihydroxyisoflavone were relatively potent, inhibiting in vivo steroid sulfatase activity by 62 and 81%, resp., at a single oral dose of 10 mg/kg. A study of the structure-activity relationship of a series of coumarin-based sulfamates has led to the development of a no. of potent non-steroidal inhibitors, one of which has a similar potency to that of EMATE. The identification of potent steroid- and non-steroid-based sulfatase inhibitors will enable the therapeutic value of this therapy to be examd. in the near future.
- IT 243129-61-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and structure-activity relationship of steroid sulfatase inhibitors)

- RN 243129-61-5 CAPLUS
- CN Sulfamic acid, 2-methoxy-4-[[[(6E)-8-methyl-1-oxo-6-nonenyl]amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

$$\begin{array}{c|c} & & & \\ &$$

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L12 ANSWER 16 OF 42 CAPLUS COPYRIGHT 2003 ACS
- AN 1999:204107 CAPLUS
- DN 131:27557
- TI Development of (p-O-sulfamoyl)-N-alkanoyl-phenylalkyl amines as non-steroidal estrone sulfatase inhibitors
- AU Kolli, Aparna; Chu, Guo-Hua; Rhodes, Michael E.; Inoue, Kengo; Selcer, Kyle W.; Li, Pui-Kai
- CS Department of Biology, Bayer School of Natural and Environmental Sciences, Duquesne University, Pittsburgh, PA, 15282, USA
- SO Journal of Steroid Biochemistry and Molecular Biology (1999), 68(1-2), 31-40
 CODEN: JSBBEZ; ISSN: 0960-0760
 - Elsevier Science Ltd.
- DT Journal
- LA English

PB

- Estrogen levels in breast tumors of postmenopausal women are as much as 10 AB times higher than estrogen levels in plasma, presumably due to in situ formation of estrogen. The major source of estrogen in breast cancer cells may be conversion of estrone sulfate to estrone by the enzyme estrone sulfatase. Thus, inhibitors of estrone sulfatase are potential agents for treatment of estrogen-dependent breast cancer. Several steroidal compds. have been developed that are potent estrone sulfatase inhibitors, most notably estrone-3-O-sulfamate. However, these compds. and their metabolites may have undesired effects, including estrogenicity. To avoid the problems assocd. with a potentially active steroid nucleus, we designed and synthesized a series of nonsteroidal estrone sulfatase inhibitors, the (p-O-sulfamoyl)-N-alkanoyl phenylalkyl amines. compds. synthesized vary in the length of their alkanoyl chain and in the no. of carbons sepg. the Ph ring and the carbonyl carbon. The ability of these compds. to inhibit estrone sulfatase activity was tested using human placental microsomes and intact cultured human breast cancer cells. Estrogenicity was also evaluated, using growth of estrogen-dependent human breast cancer cells. All of the test compds. inhibited estrone sulfatase activity of human placental microsomes to some extent, with the most effective compd. having an IC50 value of 72 nM. In general, compds. with longer alkanoyl chains (12-14 carbons) were more effective than those with shorter chains. The test compds. also inhibited estrone sulfatase activity in intact cultures of MDA-MB-231 human breast cancer cells. Again, the longer chain compds. were more effective. In both the placental and breast cancer cell sulfatase assays, the optimal distance between the Ph ring and the carbonyl carbon was 1-2 carbons. The MCF-7 cell proliferation assay revealed that estrone and estrone-3-0-sulfamate were both estrogenic, but the (p-O-sulfamoyl)-N-alkanoyl phenylalkyl amines were not. Our data indicate the utility of (p-O-sulfamoyl)-Nalkanoyl Ph alkylamines for inhibition of estrone sulfatase activity. Furthermore, our data support the concept that nonsteroidal estrone sulfatase inhibitors may be useful as therapeutic agents for estrogen-dependent breast cancers.
- IT 226950-54-5P 226950-55-6P 226950-56-7P 226950-57-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(development of (p-O-sulfamoyl)-N-alkanoyl-phenylalkyl amines as non-steroidal estrone sulfatase inhibitors)

- RN 226950-54-5 CAPLUS
- CN Sulfamic acid, 4-[[(1-oxooctyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

```
C:\STNEXP4\QUERIES\10019693 (patel - amended).str
chain nodes :
  7 8 9
ring nodes :
  1 2 3 4 5 6 10 11 12 13 14 15
```

```
chain bonds :
    2-7 7-8 8-9
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15
exact/norm bonds :
    2-7 7-8 8-9
normalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15
isolated ring systems :
    containing 1 :
```

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 16:CLASS

$$CH_2-NH-C-(CH_2)_6-Me$$
 H_2N-S-O

RN 226950-55-6 CAPLUS

CN Sulfamic acid, 4-[[(1-oxodecyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$CH_2-NH-C-(CH_2)_8-Me$$
 H_2N-S-O

RN 226950-56-7 CAPLUS

CN Sulfamic acid, 4-[[(1-oxododecyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$CH_2-NH-C-(CH_2)_{10}-Me$$
 H_2N-S-O

RN 226950-57-8 CAPLUS

CN Sulfamic acid, 4-[[(1-oxotetradecyl)amino]methyl]phenyl ester (9CI) (CA INDEX NAME)

$$CH_2-NH-C-(CH_2)_{12}-Me$$
 H_2N-S-O

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD

10/019,693 (patel)

ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/019,693 (patel)

L12 ANSWER 17 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 1999:118506 CAPLUS

DN 130:237337

TI Synthesis and sulfatase inhibitory activities of (E) - and (Z)-4-hydroxytamoxifen sulfamates

AU Chu, Guo-Hua; Peters, Amy; Selcer, Kyle W.; Li, Pui-Kai

CS Department of Medicinal Chemistry and Pharmaceutics, Mylan School of Pharmacy, Duquesne University, Pittsburgh, PA, 15282, USA

SO Bioorganic & Medicinal Chemistry Letters (1999), 9(2), 141-144 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

AB We report the development of (E)- (I) and (Z)-4-hydroxytamoxifen sulfamates as estrone sulfatase inhibitors, potential therapeutic agents for the treatment of breast cancer. Both compds. competitively inhibit estrone sulfatase isolated from rat liver with an apparent Ki of 35.9 .mu.M for I and an apparent Ki of >500 .mu.M for the Z isomer.

TT 221214-41-1P 221214-42-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and sulfatase inhibitory activity of)

RN 221214-41-1 CAPLUS

CN Sulfamic acid, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]phenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 221214-42-2 CAPLUS

CN Sulfamic acid, 4-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]phenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L12 ANSWER 18 OF 42 CAPLUS COPYRIGHT 2003 ACS
- AN 1996:169243 CAPLUS
- DN 124:316749
- N-acyl sulfamic acid esters (or thioesters), N-acyl sulfonamides, and N-sulfonyl carbamic acid esters (or thioesters) as hypercholesterolemic agents
- IN Lee, Helen T.; Picard, Joseph A.; Sliskovic, Drago R.; Wierenga, Wendell
- PA Warner-Lambert Company, USA
- SO U.S., 17 pp. Cont.-in-part of U.S. Ser. No. 62,515, abandoned. CODEN: USXXAM
- DT Patent
- LA English
- FAN.CNT 2

21200	PATENT NO.						DATE				PPLI	CATI	ON N	o. 	DATE				
ΡI	US	109431 2158268			Α		19960213			US 1994-223932				1994	0413				
										IL 1994-109431									
										CA 1994-2158268									
	WO	9426702			A1		19941124			WO 1994-US5233			3	1994	0511				
		W: A	U,	CA,	CZ,	FI,	HU,	JP,	KR,	NO,	NZ,	RU,	SK						
		RW: A																SE	
	ΑU	946831	1		A	1	1994	1212		A	J 19	94-6	8311		1994	0511			
	AU	681152			B	2	1997	0821											
		698010								E	P 19	94-9	1673	4	1994	0511			
		698010																	
		R: A																PT,	SE
	HU	08510256 178891 2133163 2137756 9403313 5633287			T2 E T3 C1		1996	50528		H	J 19	1995-2811			1994	0511			
	JΡ						19990901 19990920			J	P 19	94-5	-916734 -122768		1994	0511		•	
	ΑT									A'	г 19	94-9			1994	0511			
	ES									E	s 19	94-9			1994	19940511			
	RU									RI	J 19	95-1			1994	0511			
										ZA 1994-3313 US 1995-546967			19951023						
	US				Α		1997	L9970527											
	FI	950543	8		Α		1995	1110		F	I 19	95-5	438		1995	1110			
		O 9504564								N	19	95-4	564		19951113				
PRAI	US	1993-62515 1994-223932 1994-US5233			B	2	1993	0514											
	US				Α		19940413												
	WO				W		1994	0511											

OS MARPAT 124:316749

The present invention is directed to title ACAT-inhibiting compds. AB R1XSO2NRCOYR2 useful for the regulation of cholesterol, methods for using them and pharmaceutical compns. thereof, wherein: X and Y are oxygen, sulfur, or (CR'R'')n wherein n is 1 to 4 and R' and R'' are each independently, e.g., H, alkyl, alkoxy or R' and R'' together form a spirocycloalkyl or a carbonyl; R is hydrogen, alkyl, or benzyl; R1 and R2 are Ph, substituted Ph, naphthyl, substituted naphthyl, an aralkyl group, an alkyl chain, adamantyl, or a cycloalkyl group. Thus, e.g., hydroxyethylation of 2,6-diisopropylbromobenzene with Li/ethylene oxide afforded 2-(2,6-diisopropylphenyl)ethanol; Jones oxidn. of the latter afforded the (2,6-diisopropylphenyl)acetic acid; conversion to the acid chloride followed by amidation with 2,6-diisopropylphenyl sulfamate afforded ArcH2CONHSO2OAr (Ar = 2,6-diisopropylphenyl) which exhibited IC50 = 9.7 .mu.M for inhibition of ACAT in vitro and -63% change in mean cholesterol levels in vivo.

IT 166519-18-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(N-acyl sulfamic acid esters, N-acyl sulfonamides, and N-sulfonyl

10/019,693 (patel)

carbamic acid esters as hypercholesterolemic agents)

RN 166519-18-2 CAPLUS

CN Sulfamic acid, [1,1':3',1''-terphenyl]-2'-yl ester (9CI) (CA INDEX NAME)

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L12 ANSWER 19 OF 42 CAPLUS COPYRIGHT 2003 ACS
AN
     1995:742595 CAPLUS
DN
     123:143436
     N-acyl sulfamic acid esters (or thioesters), n-acyl sulfonamides, and
ΤI
     N-sulfonyl carbamic acid esters (or thioesters) as hypercholesterolemic
     Lee, Helen Tsenwhei; Picard, Joseph Armand; Sliskovic, Drago Robert;
IN
     Wierenga, Wendell
PA
    Warner-Lambert Co., USA
     PCT Int. Appl., 59 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 2
                                          APPLICATION NO.
     PATENT NO.
                      KIND DATE
                                                            DATE
                                          -----
                     ____
                           _____
                                          WO 1994-US5233
PΙ
                     A1
                           19941124
                                                            19940511
        W: AU, CA, CZ, FI, HU, JP, KR, NO, NZ, RU, SK
         RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
                                          US 1994-223932
                                                            19940413
     US 5491172
                           19960213
                      Α
    AU 9468311
                           19941212
                                          AU 1994-68311
                                                            19940511
                      A1
    AU 681152
                      В2
                           19970821
     EP 698010
                                          EP 1994-916734
                                                           19940511
                      A1
                           19960228
     EP 698010
                           19990414
                      В1
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
                                           JP 1994-525674
                                                            19940511
                     T2
     JP 08510256
                           19961029
                                           RU 1995-122768
                                                            19940511
     RU 2137756
                      C1
                           19990920
                                           FI 1995→5438
     FI 9505438
                      Α
                            19951110
                                                            19951110
     NO 9504564
                      Α
                            19960111
                                          NO 1995-4564
                                                            19951113
PRAI US 1993-62515
                      Α
                            19930514
                      Α
                            19940413
     US 1994-223932
                            19940511
     WO 1994-US5233
                      W
os
     MARPAT 123:143436
     Compds. of formula R1XS(O2)NRCOYR2 (R = H, C1-8 alkyl, benzyl; R1, R2 =
AB
     Ph, phenoxy, naphthyl, arylalkyl, C1-20 alkyl, etc.; X, Y = 0, S, alkyl),
     or their salts, are useful for the regulation of plasma cholesterol.
     Compds. may be used for treatment of hypercholesterolemia and
     atherosclerosis. Prepn. of 48 compds. is presented.
TТ
     166519-18-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of acyl sulfamic acid esters (or thioesters), acyl
        sulfonamides, and sulfonyl carbamic acid esters (or thioesters) as
        antihypercholesterolemic agents)
RN
     166519-18-2 CAPLUS
     Sulfamic acid, [1,1':3',1''-terphenyl]-2'-yl ester (9CI) (CA INDEX NAME)
CN
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L12 ANSWER 20 OF 42 CAPLUS COPYRIGHT 2003 ACS
AN
     1995:662328 CAPLUS
DN
     123:83996
     Preparation of amino acid derivatives as neuropeptide Y antagonists.
ΤI
     Rudolf, Klaus; Eberlein, Wolfgang; Engel, Wolfhard; Mihm, Gerhard; Doods,
IN
     Henri; Wieland, Heike-Andrea; Willim, Klaus-Dieter; Krause, Juergen;
     Dollinger, Horst; et al.
     Dr. Karl Thomae GmbH, Germany
PA
     PCT Int. Appl., 308 pp.
SO
     CODEN: PIXXD2
     Patent
DТ
     German
T.A
FAN.CNT 2
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO.
                                                            DATE
                      ____
                                                            19940118
                            19940804
                                          WO 1994-EP109
PΙ
     WO 9417035
                      A1
         W: AU, BG, BY, CA, CN, CZ, FI, HU, JP, KR, NO, NZ, PL, RO, RU, SK, UA
         RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
                          19940721
                                           DE 1993-4301452 19930120
     DE 4301452
                       A1
                            19950209
                                           DE 1993-4326465
                                                            19930806
     DE 4326465
                       A1
     AU 9458841
                       A1
                            19940815
                                           AU 1994-58841
                                                             19940118
     AU 683442
                       В2
                            19971113
                                           EP 1994-905073
                                                            19940118
     EP 680469
                       A1
                            19951108
     EP 680469
                            20000426
                       В1
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
                                           JP 1994-516636
                       T2
                                                            19940118
     JP 08505862
                            19960625
                                           AT 1994-905073
                                                             19940118
     AT 192142
                       Ε
                            20000515
                                           FI 1995-3467
     FI 9503467
                                                             19950718
                       Α
                            19950718
                                           NO 1995-2869
     NO 9502869
                       Α
                            19950919
                                                            19950719
PRAI DE 1993-4301452
                       Α
                            19930120
     DE 1993-4326465
                       Α
                            19930806
     WO 1994-EP109
                       W
                            19940118
os
     MARPAT 123:83996
     TZNR1CR2R3COY(CH2)nR [n = 0-5; R = H, OH, (substituted) Ph, naphthyl,
AΒ
     aminophenyl, aminonaphthyl, hydroxyphenyl, hydroxynaphthyl,
     diphenylmethyl, heteroaryl, cycloalkyl, etc.; Y = O, NR4; R1, R4 = H,
     alkyl, cycloalkyl, (substituted) Ph, PhCH2; R2 = substituted alkyl, Ph,
     PhCH2; R3 = H, alkyl, cycloalkyl; T = H, Ph, (substituted) heteroaryl,
     protecting group, etc.; Z = bond, CO, CH2, SO, SO2], were prepd. Thus,
     H-D-Arg(NO2)-OH in THF was treated with aq. NaOH and then with Ph2CHCOCl
     to give 85% amide. This in THF was treated with N-methylmorpholine,
     iso-Bu chloroformate, and 4-(aminomethyl)acetanilide under cooling to give
     63% (R)-N-[[4-(acetylamino)phenyl]methyl]-N5-[amino(nitroimino)methyl]-N2-
     (diphenylacetyl)ornithinamide. This was hydrogenated in aq. HOAc over Pd
     to give (R)-N-[[4-(acetylamino)phenyl]methyl]-N2-
     diphenylacetylargininamide acetate. Title compds. antagonized
     neuropeptide Y-induced effects on blood pressure in rats at 0.01-10 mg/kg.
     164643-39-4P 164645-11-8P
IT
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of amino acid derivs. as neuropeptide Y antagonists)
RN
     164643-39-4 CAPLUS
     Sulfamic acid, dimethyl-, 4-[[[5-[(aminoiminomethyl)amino]-2-
CN
     [(diphenylacetyl)amino]-1-oxopentyl]amino]methyl]phenyl ester, (R)- (9CI)
     (CA INDEX NAME)
```

Absolute stereochemistry.

RN 164645-11-8 CAPLUS

CN Sulfamic acid, dimethyl-, 4-[[[5-[(aminoiminomethyl)amino]-2-[(diphenylacetyl)amino]-1-oxopentyl]amino]methyl]phenyl ester, (R)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 164643-39-4 CMF C29 H36 N6 O5 S

Absolute stereochemistry.

CM 2

CRN 64-19-7 CMF C2 H4 O2

IT 164647-52-3P 164647-54-5P 164647-55-6P 164648-83-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of amino acid derivs. as neuropeptide Y antagonists)

RN 164647-52-3 CAPLUS

CN Carbamic acid, [1-[[[[4-[[(dimethylamino)sulfonyl]oxy]phenyl]methyl]amino] carbonyl]-4-[[imino(nitroamino)methyl]amino]butyl]-, 1,1-dimethylethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 164647-54-5 CAPLUS

CN Sulfamic acid, dimethyl-, 4-[[[2-amino-5-[[imino(nitroamino)methyl]amino]-1-oxopentyl]amino]methyl]phenyl ester, (R)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 164647-53-4 CMF C15 H25 N7 O6 S

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 164647-55-6 CAPLUS

CN Sulfamic acid, dimethyl-, 4-[[[2-[(diphenylacetyl)amino]-5-[[imino(nitroamino)methyl]amino]-1-oxopentyl]amino]methyl]phenyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 164648-83-3 CAPLUS

CN Sulfamic acid, dimethyl-, 4-(aminomethyl)phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$Me_2N-S-O$$

$$CH_2-NH_2$$

● HCl

ANSWER 21 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 1995:508003 CAPLUS

122:265364 DN

Preparation of 4-phenyloxazole and -thiazole derivatives as herbicides ΤI

Nakanishi, Hiroyuki; Miura, Juzo; Nishioka, Hitoshi; Ootsuka, Takashi IN

Nihon Nohyaku Co Ltd, Japan PA

SO Jpn. Kokai Tokkyo Koho, 47 pp.

CODEN: JKXXAF

DT Patent

LΑ Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
					-	
ΡI	JP 06340643	A2	19941213	JP 1994-89169	19940404	
PRAI	JP 1993-101921		19930404			

OS MARPAT 122:265364

The title compds. [I; R1 = halo, NO2, C1-6 alkyl, halosulfonyl, BR4, NR5; AB wherein B = 0, S(0)n (n = 0-2); R4 = H, C1-6 (halo)alkyl, C1-6hydroxyalkyl, C2-6 (halo)alkenyl, C2-6 (halo)alkynyl, C3-6 (halo)cycloalkyl, etc.; R5 = H, C1-6 (halo)alkyl, C2-6 (halo)alkenyl, C2-6 (halo)alkynyl, C3-6 cycloalkyl, C1-6 (halo)alkylsulfonyl, phenyl-C1-6 alkyl, etc.; R2 = HO, C1-6 (halo)alkyl, C1-6 cycloalkyl, C1-6 (halo)alkoxy, C1-6 alkoxy-C1-6 alkyl, C1-6 alkylthio-C1-6 alkyl; R3 = H, halo; A = O, S; X, Y = halo, C1-6 (halo)alkyl], which show excellent herbicidal activity against post- and preemergence weeds, are prepd. Thus, 3.10 g 1-bromo-2-phenyl-2-ethanone deriv. (II) and 2.61 g isobutyramide were heated at 150-160.degree. for 5.5 h to give, after silica gel chromatog., 81.9% title compd. I (R1 = iso-ProO, R2 = iso-Pr; R3 = H; X, Y = 2-F, 4-C1). I (R1 = OCH2C.tplbond.CH, R2 = iso-Pr, R3 = Iso-PrC1; X, Y = 2-F, 4-C1) at 1 kg/ha postemergence controlled .gtoreq.95% Echinochloa crus-galli in a flooded paddy soil and gave no damage to rice. A total of 165 I were prepd.

ΙT 162504-19-0P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of phenyloxazole or -thiazole deriv. as herbicide)

RN 162504-19-0 CAPLUS

Sulfamic acid, methyl-, 2-chloro-5-(5-chloro-2-propyl-4-thiazolyl)-4-CN fluorophenyl ester (9CI) (CA INDEX NAME)

L12 ANSWER 23 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 1993:516981 CAPLUS

DN 119:116981

Preparation of N-cyclohexyl-N-benzylguanidines as fungicides ΤI

Ishikawa, Hiromichi; Umeda, Ten; Hara, Takashi; Kajikawa, Kazuo IN

Hokko Chem Ind Co, Japan PA

Jpn. Kokai Tokkyo Koho, 12 pp. SO

CODEN: JKXXAF

DTPatent

LA Japanese

FAN.CNT 1

		KTND		3 2 2 7 7 2 3 M T 2 11 2 11 2	D.3.0017
	PATENT NO.		DATE	APPLICATION NO.	DATE
PΙ	JP 05058986	A2	19930309	JP 1991-240236	19910828
PRAI	JP 1991-240236		19910828		

OS MARPAT 119:116981

AB The title compds. [I; R1 = (un)substituted alkyl, alkenyl, alkynyl, alkanoyl, etc.; R2 = alkyl; R3, R4 = H, alkyl, alkenyl, alkynyl, or NR3R4 = N-contg. heterocyclyl; X = H, halo, alkyl, alkoxy] are prepd. E.g., I [R1 = X = H, R2 = Me2CH, R3 = R4 = Me] was treated with p-MeC6H4SO2Cl in THF contg. NaH at room temp. for 1 h to give the title compd. I [X = H, R1 = p-MeC6H4SO2, R2 = Me2CH, R3 = R4 = Me], which at 100 ppm showed 100%

kill of Pseudoperonospora cubensis. Many agricultural fungicidal prepns. contq. I are described.

IT 149429-65-2P 149429-71-0P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of, as fungicide)

149429-65-2 CAPLUS RN

Sulfamic acid, dimethyl-, 2-[[cyclohexyl[(dimethylamino)(phenylimino)methy CN l]amino]methyl]-4-(1-methylethyl)phenyl ester (9CI) (CA INDEX NAME)

RN 149429-71-0 CAPLUS

Sulfamic acid, diethyl-, 2-[[cyclohexyl[imino(phenylamino)methyl]amino]met CN hyl]-4-(1,1-dimethylethyl)phenyl ester (9CI) (CA INDEX NAME)

- L12 ANSWER 28 OF 42 CAPLUS COPYRIGHT 2003 ACS
- AN 1982:217218 CAPLUS
- DN 96:217218
- TI Versatile synthesis of sulfamate esters by phase-transfer methods
- AU Spillane, William J.; Taheny, Anne P.; Kearns, M. Mary
- CS Chem. Dep., Univ. Coll. Galway, Galway, Ire.
- Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1982), (3), 677-9 CODEN: JCPRB4; ISSN: 0300-922X
- DT Journal
- LA English
- AB Sulfamate esters, R2NSO3R1 (R = Me, Et), RNHSO3R1 (R = cyclohexyl), and H2NSO3R1 (R1 = alkyl, aryl) were prepd. by condensation of the appropriate sulfamoyl chloride with alcs. and phenols under mild phase-transfer conditions. E.g., reaction of Me2NSO2Cl with MeOH in C6H6 contg. PhCH2N+Et3Cl- and aq. NaOH at 50.degree. for 2 h gave 90% Me2NSO3Me. Me2NSO3R (R = Me, Et, Pr, CMe3) rearranged to the corresponding betaines Me2N+RSO3- in 95-98% yield at 130.degree..
- IT 72119-30-3P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, by condensation of sulfamoyl chloride with phenol)
- RN 72119-30-3 CAPLUS
- CN Sulfamic acid, diethyl-, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

- L12 ANSWER 29 OF 42 CAPLUS COPYRIGHT 2003 ACS
- AN 1982:199210 CAPLUS
- DN 96:199210
- TI 2-(Aminomethyl)phenols, a new class of saluretic agents. 4. Effects of oxygen and/or nitrogen substitution
- AU Stokker, G. E.; Deana, A. A.; DeSolms, S. J.; Schultz, E. M.; Smith, R. L.; Cragoe, E. J., Jr.; Baer, J. E.; Russo, H. F.; Watson, L. S.
- CS Merck Inst. Ther. Res., Merck Sharp and Dohme Res. Lab., West Point, PA, 19486, USA
- SO Journal of Medicinal Chemistry (1982), 25(6), 735-42 CODEN: JMCMAR; ISSN: 0022-2623
- DT Journal
- LA English
- AB A series of O and/or N-substituted 2-(aminomethyl)phenols was synthesized and tested orally in rats for saluretic and diuretic effects. In general, substitution on N with groups other than lower alkyl or substitution on N and/or O with groups resistant to hydrolysis substantially diminished saluretic effects.
- IT 68967-66-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and deblocking of)

- RN 68967-66-8 CAPLUS
- CN Carbamic acid, [[2-[[(dimethylamino)sulfonyl]oxy]-5-(1,1-dimethylethyl)-3-iodophenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 68967-67-9P 68967-74-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. and diuretic activity of)

- RN 68967-67-9 CAPLUS
- CN Sulfamic acid, dimethyl-, 2-(aminomethyl)-4-(1,1-dimethylethyl)-6-iodophenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & I \\ \parallel & I \\ Me_2N-S-O & \parallel \\ O & \\ H_2N-CH_2 & Bu-t \end{array}$$

● HCl

RN. 68967-74-8 CAPLUS

CN Sulfamic acid, ethyl-, 2-(aminomethyl)-4-(1,1-dimethylethyl)-6-iodophenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & I \\ \parallel & I \\ \downarrow & \downarrow \\ O & \downarrow \\ H_2N-CH_2 & Bu-t \end{array}$$

HCl

- L12 ANSWER 31 OF 42 CAPLUS COPYRIGHT 2003 ACS
- AN 1980:6189 CAPLUS
- DN 92:6189
- TI Study of the reactivity of aryl fluorosulfates with respect to secondary aliphatic amines
- AU Hedayatullah, Mir; Guy, Alain
- CS Lab. Chim. Org., Conservatoire Natl. Arts Metiers, Paris, 75141/03, Fr.
- Phosphorus and Sulfur and the Related Elements (1979), 7(1), 95-100 CODEN: PREEDF; ISSN: 0308-664X
- DT Journal
- LA French
- AB Aryl sulfamates are obtained from aryl fluorosulfates and secondary aliph. amines. The use of the HSAB concept (Hard and Soft Acids and Bases) is used to explain the difference of the reactivity between aryl fluorosulfates and aryl chlorosulfates.
- RN 72119-30-3 CAPLUS
- CN Sulfamic acid, diethyl-, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

L12 ANSWER 33 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 1978:442661 CAPLUS

DN 89:42661

TI A convenient synthesis of aryl sulfamates

AU Hedayatullah, Mir; Guy, Alain

CS Lab. Chim. Org., Conservatoire Natl. Arts Metiers, Paris, Fr.

SO Synthesis (1978), (5), 357 CODEN: SYNTBF; ISSN: 0039-7881

DT Journal

LA English

AB RnC6H5-nO3SNH2 (Rn = H, 2-, 4-Me, 2,6-Me2, 2-, 4-Ph, 4-Cl) were prepd. in 50-75% yield by NaBH4 redn. of RnC6H5-nO3SN3.

IT 25999-01-3P 67073-77-2P

RN 25999-01-3 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

RN 67073-77-2 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-2-yl ester (9CI) (CA INDEX NAME)

- L12 ANSWER 34 OF 42 CAPLUS COPYRIGHT 2003 ACS
- AN 1975:547252 CAPLUS
- DN 83:147252
- TI Synthesis and reduction of aryl azidosulfates. VI
- AU Hedayatullah, Mir; Guy, Alain
- CS Lab. Chim. Org. Appl., Conservatoire Natl. Arts Metiers, Paris, Fr.
- SO Tetrahedron Letters (1975), (29), 2455-8 CODEN: TELEAY; ISSN: 0040-4039
- DT Journal
- LA French
- AB Reaction of p-RC6H4OSO2Cl (R = H, Me, Cl, Ph) with NaN3 in MeCN gave 90-8% p-RC6H4OSO2N3 (I) which in MeOH with powd. Cu gave 47-86% p-RC6H4OSO2NH2. LiAlH4 redn. of I gave the corresponding phenols by cleavage of the O-S bond.
- IT 25999-01-3P

- RN 25999-01-3 CAPLUS
- CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

L12 ANSWER 35 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 1972:539511 CAPLUS

DN 77:139511

TI Preparation and reactions of aryloxysulfonyl isocyanates

AU Lohaus, Gerhard

CS Farbwerke Hoechst A.-G., Frankfurt/M., Fed. Rep. Ger.

SO Chemische Berichte (1972), 105(9), 2791-9 CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

Re-action of phenols ROH (e.g. R = Ph, p-MeC6H4, m-ClC6H4, 2,4,6-Cl3C6H2, p-NCC6H4) with ClSO2NCO gave 40-79% ROSO2NCO (I). Hydrolysis of I yielded nearly quant. ROSO2NH2 (II). I are highly active compds. and the reactivity corresponded to the acidity of the starting phenols. II was useful for the transfer of SO2NH2 groups, e.g. to amines.

IT 25999-01-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 25999-01-3 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

L12 ANSWER 36 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 1971:127560 CAPLUS

DN 74:127560

TI 3-Substituted-7-aminocoumarins, as optical brighteners or their intermediates

PA Farbenfabriken Bayer A.-G.

SO Fr. Demande, 12 pp.

CODEN: FRXXBL

DT Patent

LA French

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI FR 2016308

19700508

PRAI DE

19680823

AB Title compds. (I) are prepd. by heating the corresponding 5,2,4-R1(RO)(H2N)C6H2CH:C(R2)CN (II, R = SO2NMe2 or CH2OMe) (cf. Fr. Demande 2,016,307) with aq. mineral acids at 104-55.degree. for 6-10 hr. Thus II (R1 = H, R2 = Ph, R = Me2NSO2) was heated in 62% H2SO4 at 130.degree. for 7 hr to give I (R1 = H, R2 = Ph). Similarly 10 other I were prepd.

TT 31804-41-8P 31804-42-9P 31804-43-0P 31804-44-1P 31804-45-2P 31804-51-0P

RN 31804-41-8 CAPLUS

CN Sulfamic acid, dimethyl-, ester with 3-(4-amino-2-hydroxyphenyl)-2-phenylacrylonitrile (8CI) (CA INDEX NAME)

RN 31804-42-9 CAPLUS

CN Sulfamic acid, dimethyl-, ester with 3-(4-amino-2-hydroxyphenyl)-2-p-tolylacrylonitrile (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & O & \\ S-NMe_2 \\ \hline \\ C & CH \end{array}$$

RN 31804-43-0 CAPLUS

CN Sulfamic acid, dimethyl-, ester with 3-(4-amino-2-hydroxyphenyl)-2-(p-methoxyphenyl)acrylonitrile (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \text{CN} & \text{NH}_2 \\ \hline & \text{C} & \text{CH} & \text{O} \\ \hline & \text{O} & \text{S-NMe}_2 \\ \hline & \text{O} & \text{O} \end{array}$$

RN 31804-44-1 CAPLUS

CN Sulfamic acid, dimethyl-, ester with 3-(4-amino-2-hydroxyphenyl)-2-(p-chlorophenyl)acrylonitrile (8CI) (CA INDEX NAME)

RN 31804-45-2 CAPLUS

CN Sulfamic acid, dimethyl-, ester with 3-(4-amino-2-hydroxyphenyl)-2-(3,4-dichlorophenyl)acrylonitrile (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 & CN & NH_2 \\ \hline C - CH & O & \\ \hline C1 & O & S-NMe_2 \\ \hline \\ O & O & O & S-NMe_2 \\ \hline \\ O & O & S-NMe_2 \\ \hline \\ O & O & O & O \\ \hline \\ O & O & O & O \\ \hline \\ O & O & O & O \\ \hline \\ O & O & O & O \\ \hline \\ O$$

RN 31804-51-0 CAPLUS

CN Sulfamic acid, dimethyl-, ester with 3-(4-amino-6-hydroxy-m-tolyl)-2-phenylacrylonitrile (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & \\ \parallel & \\ O - S - NMe_2 \\ \parallel & \\ O \\ CH \longrightarrow C - CN \\ \downarrow \\ Ph \end{array}$$

L12 ANSWER 37 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 1971:113267 CAPLUS

DN 74:113267

TI Substituted .beta.-phenylacrylonitrile derivatives as intermediates for optical brighteners

PA Farbenfabriken Bayer A.-G.

SO Fr. Demande, 13 pp.

CODEN: FRXXBL

DT Patent

LA French

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI FR 2016307

19700508 19680823

PRAI DE

5,2,4-R1(RO)(O2N)C6H2Me are treated with Na2Sx in ROH or Me2SO at 50-120.degree. 0.5-3 hr to give 5,2,4-R1-(RO)(H2N)C6H2CHO, which react with R2CH2CN at 20-120.degree. to give the title products (I) which can be converted into the corresponding coumarins by heating with aq. mineral acid at 80-200.degree. (cf. Fr. Demande 2,016,308). Thus, an aq. soln. of Na2S, NaOH, and S was added dropwise to a boiling aq. alc. soln. of 2,4-MeO(O2N)C6H3Me, the mixt. boiled for 0.5 hr, treated with PhCH2CN, and boiled for 1 hr to give I (R = Me, R1 = H, R2 = Ph). Similarly, 16 other I were prepd.

IT 31804-41-8P 31804-42-9P 31804-43-0P 31804-44-1P 31804-45-2P 31804-51-0P

RL: IMF (Industrial manufacture); PREP (Preparation)

(prepn. of)

RN 31804-41-8 CAPLUS

CN Sulfamic acid, dimethyl-, ester with 3-(4-amino-2-hydroxyphenyl)-2-phenylacrylonitrile (8CI) (CA INDEX NAME)

$$Me_2N - S \longrightarrow O \qquad Ph$$

$$O \qquad CH \longrightarrow C - CN$$

$$H_2N$$

RN 31804-42-9 CAPLUS

CN Sulfamic acid, dimethyl-, ester with 3-(4-amino-2-hydroxyphenyl)-2-p-tolylacrylonitrile (8CI) (CA INDEX NAME)

RN 31804-43-0 CAPLUS

CN Sulfamic acid, dimethyl-, ester with 3-(4-amino-2-hydroxyphenyl)-2-(p-methoxyphenyl)acrylonitrile (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \text{CN} & \text{NH}_2 \\ \hline & \text{C} & \text{CH} & \text{O} \\ \hline & \text{O} & \text{S} - \text{NMe}_2 \\ \hline & \text{O} & \text{O} \end{array}$$

RN 31804-44-1 CAPLUS

CN Sulfamic acid, dimethyl-, ester with 3-(4-amino-2-hydroxyphenyl)-2-(p-chlorophenyl)acrylonitrile (8CI) (CA INDEX NAME)

RN 31804-45-2 CAPLUS

CN Sulfamic acid, dimethyl-, ester with 3-(4-amino-2-hydroxyphenyl)-2-(3,4-dichlorophenyl)acrylonitrile (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & NH_2 \\ \hline C & CH & O \\ \hline C1 & C & S-NMe_2 \\ \hline O & O & O & S-NMe_2 \\ \hline O & O & O & S-NMe_2 \\ \hline O & O & O & S-NMe_2 \\ \hline O & O & O & O \\ \hline O & O & O & O \\ \hline O & O & O & O \\ \hline O & O & O & O \\ \hline O & O & O & O \\ \hline O$$

RN 31804-51-0 CAPLUS

CN Sulfamic acid, dimethyl-, ester with 3-(4-amino-6-hydroxy-m-tolyl)-2-phenylacrylonitrile (8CI) (CA INDEX NAME)

L12 ANSWER 38 OF 42 CAPLUS COPYRIGHT 2003 ACS

AN 1970:55051 CAPLUS

DN 72:55051

TI Sulfamic acid aryl esters

PA Farbwerke Hoechst A.-G

SO Fr., 3 pp.

CODEN: FRXXAK

DT Patent

LA French

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI FR 1554976

19690124

PRAI DE

19670128

Isocyanates Ar(OSO2NCO)n (where Ar = aryl, n = 1 or 2) (Ger. 1,230,017) AΒ react with H2O to yield aryl sulfamate N-carboxylic acids which lose CO2 spontaneously to form Ar(OSO2NH2)n (I). Thus, 15 g H2O is added dropwise to 64 g 4-NCC6H4OSO2NCO in 500 ml CCl4 to ppt. 55 g 4-NCC6H4-OSO2NH2, m. 155.degree.. Other I (n = 1) prepd. are the following (Ar and m.p. qiven): 4-ClC6H4, 105.degree.; 3-ClC6H4, 80.degree.; Ph, 86.degree.; 4-MeC6H4, 80.degree.; 3-MeC6H4, 88.degree.; 2,6-Me2C6H3, 110.degree.; 2,3-Me2-C6H3, 78.degree.; 2,5-Me2C6H3, 104.degree.; 2,4,5-Cl3C6H2 (II), 158.degree.; 2,4,6-Cl3C6H2, 144.degree.; 2,4,6-Br3C6H2, 164.degree.; C6C15, 215.degree.; 4-MeO-C6H4, 165.degree.; 4-PhN2C6H4, 160.degree.; the sulfonate of 3-hydroxydibenzofuran, 156.degree.; and hydroquinone bis(sulfamate), 200.degree.. The compds. are useful for transferring the sulfonamide group. Thus, by shaking 1.35 g II with 0.9 g morpholine in 5 ml CH2Cl2, the ester dissolves to yield 0.71 g morpholine-N-sulfonamide, m. 160.degree..

IT 25999-01-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 25999-01-3 CAPLUS

CN Sulfamic acid, [1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

L12 ANSWER 39 OF 42 CAPLUS COPYRIGHT 2003 ACS AN 1965:43634 CAPLUS DN 62:43634 OREF 62:7670a-c Synthesis and anticholinesterase activity of a series of aryl N, N-dimethylsulfamates ΑU Corral, C.; Municio, A. M. CS Inst. Quim., Madrid SO Anales Real Soc. Espan. Fis. Quim. (Madrid) (1964), Ser. B 60(4), 341-4 DTJournal LΑ Unavailable AΒ A series of N,N-dimethylsulfamates was prepd. Thus, 0.03 mole corresponding phenol was exactly neutralized with 2N NaOH and the soln. evapd. to dryness on a steam bath in vacuo. To the dry phenolate was added 50 ml. anhyd. EtCOMe and 0.03 mole MeNSO2Cl and the mixt. rerefluxed 8 hrs. to give the following aryl N,N-dimethylsulfamates [aryl group and m.p. and (or) b.p./mm. given]: 1-naphthyl, 77.degree., 90.degree./0.1; 2-naphthyl, 73.degree.; 2-cyclohexylphenyl, 62.degree.; 2-phenylphenyl, 78.degree.; 3-methylcoumaryl, 151.degree.; 3-pyridyl, 99.degree./0.25; 2-methylphenyl, 95.degree./0.1; 3-methylphenyl, 94.degree./0.1; 4-methylphenyl, 95.degree./0.1; 2-methoxyphenyl, 38-42.degree., 120.degree./0.5; 3-methoxyphenyl, 124.degree./0.1; 4-methoxyphenyl, 140.degree./1; 2-isopropoxyphenyl, 125.degree./0.5; 2-chlorophenyl, 38.degree., 98.degree./0.05; 3-chlorophenyl, 105.degree./0.1; 4-chlorophenyl, 46.degree., 102.degree./0.5; 2-nitrophenyl, 66.degree.; 3-nitrophenyl, 85.degree.; 4-nitrophenyl, 124.degree.; 2-carbethoxyphenyl, 128.degree./0.1; 3-carbethoxyphenyl, 130.degree./0.05; 4-carbethoxyphenyl, 136.degree./0.1; 3-ethyl-5-methylphenyl, 124.degree./0.5; carvacryl, 122.degree./0.05; isothymyl, 105.degree./0.1; thymyl, 108.degree./0.1; 3,5-dichlorophenyl, 106.degree./0.1; 3,4-dichlorophenyl, 60.degree.; 2,3-dichlorophenyl, 73.degree.; 4-chloro-3-methylphenyl, 28.degree.; 4-nitro-3-methylphenyl, 67.degree.; 2,4,5-trichlorophenyl, 85.degree.; 2,3,5-trimethylphenyl, 72.degree.; 4,6-dichloro-3-methylphenyl, 118.degree./0.1. None of the esters showed anticholinesterase activity at 10-3M concn. The 3,5-dichlorophenyl, 4-chlorophenyl, 3,4-dichlorophenyl, 3-chlorophenyl, and Ph esters showed, in decreasing order, the greatest insecticidal activity. The rest were much less active. 1151-28-6, Sulfamic acid, dimethyl-, 2-biphenylyl ester ΙT (anticholinesterase activity of) RN 1151-28-6 CAPLUS Sulfamic acid, dimethyl-, 2-biphenylyl ester (7CI, 8CI) (CA INDEX NAME) CN

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L12 ANSWER 42 OF 42 CAPLUS COPYRIGHT 2003 ACS
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AN 1963:408988 CAPLUS

DN 59:8988

OREF 59:1636b-f

TI N, N-Bis-(2-chloroethyl) sulfoamines

AU Preussmann, Rudolf

SO Arzneimittel-Forsch. (1962), 12, 1119-23

DT Journal

LA Unavailable

AΒ The prepn. of 21 derivs. of N,N-bis(2-chloroethyl)sulfoamines, which are nitrogen mustard derivs. of sulfuric acid, was reported. The lability of chlorine and the therapeutic effect on the transplanted Yoshida sarcoma in rats was detd. and correlations between the chem. structure and biol. effects were discussed. To a soln. of 36 g. COCl2 in 300 ml. C6H6 was added a soln. of bis(2-chloroethyl)-amine, prepd. from 70 g. HCl salt, and 54 ml. Et3N dropwise, with cooling and stirring at 10.degree.. The mixt. was kept 2 hrs. at room temp., Et3N.HCl filtered off, the C6H6 soln. washed with ag. acid, NaHCO3, and H2O, and dried with Na2SO4 to give Z2NCOC1 (Z = C1CH2CH2 throughout abstr.) (I), b2 118.degree. (81% yield). I (150 g.) was treated with 59 g. SO3 3 hrs. at room temp. and warmed on a water bath at 80.degree. to remove CO2. The mixt. was extd. with Et2O and the ext. washed with NaHCO3 and H2O to give 158 g. Z2NSO2Cl (II), b5 126.degree.. II treated with NaOMe gave 83% Z2NSO3Me, b4 143-5.degree.. II and NaOPh gave Z2NSO3-Ph. Diethylstilbestrol (4.5 g.) was treated with a soln. of 0.8 q. Na in 40 ml. MeOH, refluxed 10 min., and pptd. with H2O to give (p-Z2NSO3CEt:)2 (6 g.), m. 122-4.degree.(MeOH). II (33 g.) was treated with 6 q. NH3 in 600 ml. dioxane, the mixt. held overnight at room temp., and NH4Cl filtered off to give 45% Z2NSO2-NH2, m. 82.5-3.5.degree.. Glycine ester (5.2 g.), 6.9 ml. Et3N, and 12 g. II in 50 ml. dioxane was kept overnight at room temp. to give after filtration of Et3N.HCl 9 g. Z2NSO2NHCH2CO2Et, m. 61-3.degree. (aq. EtOH). Similarly were prepd. (Z2NSO2NHCH2)2, m. 75.degree., [Z2NSO2NH(CH2)3]2, m. 124.degree. (EtOH), Z2NSO2NEt2, oil; Z2NSO2NZ2, oil; IIa, m. 138.5-9.5.degree. (EtOH), Z2NSO2NHNH2 (III), m. 100-1.degree. (Et20-petr. ether); HCl salt m. 116-18.degree.. III (23.6 g.) refluxed with 0.1 mole of aldehyde or ketone in Et20 2 hrs. yielded 60-90% of the hydrazone Z2NSO2NHN:R (R and m.p. given): Me2C, 81.5.degree.; MeCCH2CO2Et, 75-6.degree.; MeCCH2CH2CO2H, 117-18.degree.; HOCH2(CH2OH)4CH(from glucose), 65-70.degree.; MeCAc, 76.5-7.5.degree.; p-Me2NC6H4CH, 144.5-5.5.degree. (oxalate m. 155-5.5.degree.); 3-methylenepyridine, 121-2.degree. (HCl salt 132-3.degree.). Acetylacetone (2 g.) in 5 ml. EtOH was added to 5.5 g. III in 15 ml. 2N HCl and 10 ml. EtOH at 0.degree. to give IV. Also prepd. was (Z2NSO2NHN:CMe)2, m. 167.5-8.5.degree.. The lability of chlorine was detd. of a 0.23M soln. in dioxane with 6M NaHCO3 at 37.degree.. ΙT 102584-76-9, Sulfamic acid, bis(2-chloroethyl)-, diester with

RN 102584-76-9 CAPLUS

(prepn. of)

CN Sulfamic acid, bis(2-chloroethyl)-, (1,2-diethyl-1,2-ethenediyl)di-4,1-phenylene ester (9CI) (CA INDEX NAME)

.alpha.,.alpha.'-diethyl-4,4'-stilbenediol

=> d his

(FILE 'HOME' ENTERED AT 14:11:00 ON 13 MAY 2003)

	FILE	'REGIS	TRY'	ENTERED	AT 14:3	11:07	ON 13	3 MA	Y 2003				
L1			STRUC	TURE UP	LOADED								
L2		50	S L1	SSS SAM									
L3			SCREE	N 2016 (OR 2026	OR	2039	OR	2040 C	R	2045	OR	2047
L4			STRUC	TURE UP	LOADED								
L5			QUE L	4 NOT L	3								
L6		50	S L5	SSS SAM									
L7			SCREE	N 2016 (OR 2026	or or	2039	OR	2040 C	R	2045	OR	2047
L8			STRUC	TURE UP	LOADED								
L9			QUE L	8 NOT L	7								
L10		10	S L9	SSS SAM									
L11		255	S L9	SSS FUL									
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FILE 'CAPLUS' ENTERED AT 14:26:49 ON 13 MAY 2003
2 42 S L11

FILE 'CAOLD' ENTERED AT 14:28:03 ON 13 MAY 2003

=> s 111

L13 4 L11

=> d 113 1-4 bib,hitstr

L13 ANSWER 1 OF 4 CAOLD COPYRIGHT 2003 ACS

AN CA62:7670a CAOLD

TI synthesis and anticholinesterase activity of a series of aryl N,N-dimethylsulfamates

AU Corral, C.; Martin Municio, A.

IT 1151-28-6

RN 1151-28-6 CAOLD

CN Sulfamic acid, dimethyl-, 2-biphenylyl ester (7CI, 8CI) (CA INDEX NAME)

L13	ANSWER 2 OF 4 CAOLD COPYRIGHT 2003 ACS							
AN	CA59:3853b CAOLD							
TI	aromatic carboxylic acids							
AU	Juettner, Bernhard; Benning, A.							
DT	Patent							
TI	carboxylic acids (aromatic)							
PA	Bergwerksverband G.m.b.H.							
DΤ	Patent							
	PATENT NO. KIND DATE							
ΡI	DE 1136687							

IT 101547-37-9

101547-37-9 CAOLD RN

Sulfamic acid, dipropyl-, 4,4'-biphenylylene ester (7CI) (CA INDEX NAME) CN

L13 AN TI	ANSWER 3 OF 4 CAOLD COP CA59:3852g CAOLD aryl dialkylsulfamates	YRIGHT 2003 ACS	
AU	Dunbar, Joseph E.		
PA	Dow Chemical Co.		
DT	Patent		
	PATENT NO. KIND	DATE	
PI ~	US 3082238	1963	
ΙT	98176-69-3		
RN	98176-69-3 CAOLD		
CN	Sulfamic acid, dimethyl-,	4,4'-biphenylylene ester (7CI)	(CA INDEX NAME)

$$\begin{array}{c|c} O & O & O \\ Me_2N-S-O & O-S-NMe_2 \\ O & O & O \end{array}$$

- L13 ANSWER 4 OF 4 CAOLD COPYRIGHT 2003 ACS
- AN CA59:1636b CAOLD
- TI N, N-bis-(2-chloroethyl) sulfoamines
- AU Preussmann, Rudolf
- IT 102584-76-9
- RN 102584-76-9 CAOLD
- CN Sulfamic acid, bis(2-chloroethyl)-, (1,2-diethyl-1,2-ethenediyl)di-4,1-phenylene ester (9CI) (CA INDEX NAME)

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